Hexanedioic acid, bis(2-ethylhexyl) ester

Other names:

ADO (lubricating oil)
Adimoll DO
Adipic acid di(2-ethylhexyl) ester
Adipic acid, bis(2-ethylhexyl) ester
Adipol 2EH
BEHA
Bis(2-ethylhexyl) adipate
Bis(2-ethylhexyl) hexanedioate
Bis-(2-ethylhexyl)ester kyseliny adipove
Bis-(2-ethylhexyl)ester kyseliny adipove (czech)
Bisoflex DOA
Crodamol DOA
DEHA
DOA
Di(2-ethylhexyl) adipate
Diethylhexyl adipate
Dioctyl adipate
Effomoll DOA
Ergoplast Addo
Flexol A 26
Flexol plasticizer 10-A
Flexol plasticizer A-26
Good-rite GP-223
Hatcol 2908
Hexanedioic acid, 1,6-bis(2-ethylhexyl) ester
Jayflex DOA 2
K 3220
Kemester 5652
Kodaflex DOA
Lankroflex DOA
Mollan S
Monoplex DOA
Monsanto DOA
NCI-C54386
PX-238
Palatinol DOA
Plasthall DOA
Plastomoll DOA
Polycizer DOA
Reomol DOA

Rucoflex plasticizer doa
Sansocizer DOA
Sicol 250
Staflex doa
Truflex DOA
Uniflex doa
Vestinol OA
WITAMOL 320
Wickenol 158
diacizer DOA
effomoll DA
hexanedioic acid bis(2-ethylhexyl) ester
octyl adipate

Inchi: InChI=1S/C22H42O4/c1-5-9-13-19(7-3)17-25-21(23)15-11-12-16-22(24)26-18-20(8-4)14

InchiKey: SAOKZLXYCUGLFA-UHFFFAOYSA-N

Formula: C22H42O4

SMILES: CCCCC(CC)COC(=O)CCCCC(=O)OCC(CC)CCCC

Mol. weight [g/mol]: 370.57

CAS: 103-23-1

Physical Properties

Property code	Value	Unit	Source
gf	-338.36	kJ/mol	Joback Method
hf	-997.57	kJ/mol	Joback Method
hfus	51.26	kJ/mol	Joback Method
hvap	82.10	kJ/mol	Joback Method
log10ws	-5.06		Aqueous Solubility Prediction Method
logp	6.066		Crippen Method
mcvol	335.720	ml/mol	McGowan Method
pc	963.27	kPa	Joback Method
rinpol	2382.00		NIST Webbook
rinpol	2381.00		NIST Webbook
rinpol	2390.00		NIST Webbook
rinpol	2383.00		NIST Webbook
rinpol	2398.20		NIST Webbook
rinpol	2361.00		NIST Webbook
rinpol	2381.00		NIST Webbook
rinpol	2381.00		NIST Webbook
rinpol	2383.00		NIST Webbook

rinpol	2382.00		NIST Webbook
rinpol	2382.00		NIST Webbook
ripol	1896.00		NIST Webbook
ripol	1892.00		NIST Webbook
ripol	1892.00		NIST Webbook
sl	865.00	J/mol×K	NIST Webbook
tb	854.46	K	Joback Method
tc	1046.57	K	Joback Method
tf	161.50	K	NIST Webbook
tf	205.75	K	Aqueous Solubility Prediction Method
vc	1.304	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1112.15	J/mol×K	886.48	Joback Method
cpg	1190.16	J/mol×K	1046.57	Joback Method
cpg	1176.86	J/mol×K	1014.55	Joback Method
cpg	1162.43	J/mol×K	982.53	Joback Method
cpg	1146.85	J/mol×K	950.51	Joback Method
cpg	1130.10	J/mol×K	918.50	Joback Method
cpg	1092.98	J/mol×K	854.46	Joback Method
cpl	701.50	J/mol×K	300.00	NIST Webbook
dvisc	0.0003731	Pa×s	519.09	Joback Method
dvisc	0.0001845	Pa×s	586.17	Joback Method
dvisc	0.0001055	Pa×s	653.24	Joback Method
dvisc	0.0000669	Pa×s	720.31	Joback Method
dvisc	0.0000458	Pa×s	787.39	Joback Method
dvisc	0.0009298	Pa×s	452.02	Joback Method
dvisc	0.0000333	Pa×s	854.46	Joback Method
sdco	0.00	m2/s	338.47	Self-diffusivity measurements of dimethyl, diethyl, dipropyl, dibutyl, Bis(2-ethylhexyl) adipates from (293 - 339) K by a PGSE-NMR spin-echo technique

sdco	0.00	m2/s	329.45	Self-diffusivity measurements of dimethyl, diethyl, dipropyl, dibutyl, Bis(2-ethylhexyl) adipates from (293 - 339) K by a PGSE-NMR spin-echo technique
sdco	0.00	m2/s	320.46	Self-diffusivity measurements of dimethyl, diethyl, dipropyl, dibutyl, Bis(2-ethylhexyl) adipates from (293 - 339) K by a PGSE-NMR spin-echo technique
sdco	0.00	m2/s	311.45	Self-diffusivity measurements of dimethyl, diethyl, dipropyl, dibutyl, Bis(2-ethylhexyl) adipates from (293 - 339) K by a PGSE-NMR spin-echo technique
sdco	0.00	m2/s	302.44	Self-diffusivity measurements of dimethyl, diethyl, dipropyl, dibutyl, Bis(2-ethylhexyl) adipates from (293 - 339) K by a PGSE-NMR spin-echo technique
sdco	0.00	m2/s	293.43	Self-diffusivity measurements of dimethyl, diethyl, dipropyl, dibutyl, Bis(2-ethylhexyl) adipates from (293 - 339) K by a PGSE-NMR spin-echo technique

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	440.20	K	0.10	NIST Webbook

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
293.15	100.00	925.4
293.15	2510.00	926.9
293.15	5000.00	928.4
293.15	5010.00	928.4
293.15	7550.00	929.9
293.15	10010.00	931.3
293.15	15040.00	934.2
293.15	20020.00	937.0
293.15	30030.00	942.4
293.15	40010.00	947.4
293.15	50020.00	952.3
293.15	68030.00	960.4
313.15	100.00	910.3
313.15	2530.00	911.9
313.15	2540.00	911.9
313.15	5020.00	913.5
313.15	7540.00	915.2
313.15	10010.00	916.7
313.15	15010.00	919.8
313.15	20000.00	922.8
313.15	30030.00	928.7
313.15	40020.00	934.1
313.15	50010.00	939.3
313.15	68050.00	947.9
333.15	100.00	895.3
333.15	2500.00	897.1
333.15	2500.00	897.1
333.15	5000.00	898.8
333.15	7480.00	900.6
333.15	9990.00	902.3
333.15	14990.00	905.7
333.15	19970.00	908.9
333.15	30010.00	915.2
333.15	39990.00	921.0
333.15	50020.00	926.6

333.15	68010.00	935.8
353.15	100.00	880.4
353.15	2510.00	882.3
353.15	2500.00	882.3
353.15	5000.00	884.2
353.15	7510.00	886.1
353.15	10000.00	888.0
353.15	15010.00	891.7
353.15	20020.00	895.2
353.15	30030.00	902.0
353.15	40020.00	908.2
353.15	50010.00	914.1
353.15	68010.00	923.9
373.15	100.00	865.4
373.15	2510.00	867.5
373.15	2510.00	867.5
373.15	5020.00	869.7
373.15	7510.00	871.7
373.15	10010.00	873.8
373.15	14990.00	877.8
373.15	20000.00	881.6
373.15	30010.00	888.9
373.15	40000.00	895.6
373.15	50010.00	901.9
373.15	68000.00	912.3
293.15	100.00	925.4
293.15	5000.00	928.3
293.15	10020.00	931.3
293.15	20020.00	937.0
293.15	40020.00	947.4
293.15	68030.00	960.3

Reference *https://www.doi.org/10.1016/j.fluid.2014.04.018*

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103231&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Density measurements of compressed dipropyl, dibutyl, bis(2-ethylhexyl) adipates from (293 to 373 K) at pressures up to about 68 MPa:	https://www.doi.org/10.1016/j.fluid.2014.04.018
Self-diffusivity measurements of dimethyl, diethyl, dipropyl, dibutyl, Bis(2-ethylhexyl) adipates from (293 - 339) K by a PGSE-NMR spin-echo technique:	https://www.doi.org/10.1016/j.fluid.2015.11.020

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sdco:	Self diffusion coefficient
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume