Hexanedioic acid, dioctyl ester

Other names:	Adiimoll DO
	Dioctyl adipate
	Dioctyl ester of hexanedioic acid
	Dioctyl hexanedioate
	Hexanedioic acid, 1,6-dioctyl ester
	NSC 16201
	Octyl adipate
	adimoll DO
	adipic acid, dioctyl ester
	di-n-octyl adipate
	hexanedioic acid dioctyl ester
Inchi:	InChI=1S/C22H42O4/c1-3-5-7-9-11-15-19-25-21(23)17-13-14-18-22(24)26-20-16-12-10-
InchiKey:	NEHDRDVHPTWWFG-UHFFFAOYSA-N
Formula:	C22H42O4
SMILES:	CCCCCCCCOC(=O)CCCCC(=O)OCCCCCCCC
Mol. weight [g/mol]:	370.57
CAS:	123-79-5

Physical Properties

Property code	Value	Unit	Source
gf	-333.48	kJ/mol	Joback Method
hf	-987.01	kJ/mol	Joback Method
hfus	58.31	kJ/mol	Joback Method
hvap	82.88	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	6.354		Crippen Method
mcvol	335.720	ml/mol	McGowan Method
pc	953.78	kPa	Joback Method
rinpol	398.20		NIST Webbook
rinpol	398.20		NIST Webbook
rinpol	398.20		NIST Webbook
ripol	2846.00		NIST Webbook
ripol	2834.00		NIST Webbook
ripol	2846.00		NIST Webbook
ripol	2846.00		NIST Webbook
ripol	2834.00		NIST Webbook
tb	855.34	K	Joback Method

tc	1047.20	K	Joback Method
tf	482.02	K	Joback Method
vc	1.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1092.06	J/mol×K	855.34	Joback Method
cpg	1111.23	J/mol×K	887.32	Joback Method
cpg	1129.19	J/mol×K	919.29	Joback Method
cpg	1145.99	J/mol×K	951.27	Joback Method
cpg	1161.63	J/mol×K	983.25	Joback Method
cpg	1176.14	J/mol×K	1015.23	Joback Method
cpg	1189.55	J/mol×K	1047.20	Joback Method
dvisc	0.0006693	Pa×s	482.02	Joback Method
dvisc	0.0003195	Pa×s	544.24	Joback Method
dvisc	0.0001775	Pa×s	606.46	Joback Method
dvisc	0.0001100	Pa×s	668.68	Joback Method
dvisc	0.0000739	Pa×s	730.90	Joback Method
dvisc	0.0000529	Pa×s	793.12	Joback Method
dvisc	0.0000397	Pa×s	855.34	Joback Method
hvapt	99.00	kJ/mol	433.00	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123795&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Liquid-Liquid Equilibria of Formic Acid and Furfural in a Biphasic Aqueous-Organic System: Optimization of Solvent and Amine Extractant:	https://www.doi.org/10.1021/acs.jced.8b00335

Legend

cpg:	Ideal gas 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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume