Decanedioic acid, dihexyl ester

Other names: Di-n-hexyl sebacate
dihexyl decanedioate
dihexyl sebacate
Inchi: InChI=1S/C22H42O4/c1-3-5-7-15-19-25-21(23)17-13-11-9-10-12-14-18-22(24)26-20-16-
InchiKey: GQIDSVPVVYHXAP-UHFFFAOYSA-N
Formula: C22H42O4
SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)OCCCCCC
Mol. weight [g/mol]: 370.57
CAS: 2449-10-7

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	106.40 ± 3.70	kJ/mol	NIST Webbook
log10ws	-4.57		Aqueous Solubility Prediction Method
logp	6.354		Crippen Method
mcvol	335.720	ml/mol	McGowan Method
pc	953.78	kPa	Joback Method
tb	855.34	K	Joback Method
tc	1047.20	K	Joback Method
tf	274.00	K	NIST Webbook
vc	1.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1176.14	J/mol×K	1015.23	Joback Method
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	1189.55	J/mol×K	1047.20	Joback Method
cpl	711.00	J/mol×K	303.15	NIST Webbook
cpl	732.00	J/mol×K	315.00	NIST Webbook
dvisc	0.0000397	Pa×s	855.34	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
hvapt	99.90	kJ/mol	344.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2449107&Units=SI

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

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

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

Latest version available from:
https://www.chemeo.com/cid/43-203-8/Decanedioic-acid-dihexyl-ester.pdf
Generated by Cheméo on 2024-04-26 18:46:39.577998987 +0000 UTC m=+16446448.498576302.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.