didodecyl sebacate

Other names: Di-n-dodecyl sebacate
Inchi: InChI=1S/C34H66O4/c1-3-5-7-9-11-13-15-19-23-27-31-37-33(35)29-25-21-17-18-22-26-
InchiKey: HIKZOIYUQFYFBB-UHFFFAOYSA-N
Formula: C34H66O4
SMILES: CCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCCCCCCCCCCC
Mol. weight [g/mol]: 538.89
CAS: 2432-88-4

Physical Properties

Property code	Value	Unit	Source
gf	-232.44	kJ/mol	Joback Method
hf	-1234.69	kJ/mol	Joback Method
hfus	89.39	kJ/mol	Joback Method
hvap	154.50 ± 5.40	kJ/mol	NIST Webbook
log10ws	-11.78		Crippen Method
logp	11.035		Crippen Method
mcvol	504.800	ml/mol	McGowan Method
pc	518.88	kPa	Joback Method
tb	1129.90	K	Joback Method
tc	1472.40	K	Joback Method
tf	617.26	K	Joback Method
vc	1.988	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1869.04	J/mol×K	1129.90	Joback Method
cpg	1897.14	J/mol×K	1186.98	Joback Method
cpg	1921.20	J/mol×K	1244.07	Joback Method
cpg	1941.52	J/mol×K	1301.15	Joback Method
cpg	1958.38	J/mol×K	1358.23	Joback Method
cpg	1972.09	J/mol×K	1415.31	Joback Method
cpg	1982.95	J/mol×K	1472.40	Joback Method
cpl	1117.00	J/mol×K	368.00	NIST Webbook

dvisc	0.0001351	Pa×s	617.26	Joback Method
dvisc	0.0000585	Pa×s	702.70	Joback Method
dvisc	0.0000304	Pa×s	788.14	Joback Method
dvisc	0.0000179	Pa×s	873.58	Joback Method
dvisc	0.0000116	Pa×s	959.02	Joback Method
dvisc	0.0000081	Pa×s	1044.46	Joback Method
dvisc	0.0000059	Pa×s	1129.90	Joback Method
hvapt	131.90	kJ/mol	420.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C2432884&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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