

Sebacic acid, heptadecyl 2-methoxyethyl ester

Inchi:	InChI=1S/C30H58O5/c1-3-4-5-6-7-8-9-10-11-12-13-14-17-20-23-26-34-29(31)24-21-18-
InchiKey:	BPVTUZXGILRDKV-UHFFFAOYSA-N
Formula:	C30H58O5
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCCCCCC(=O)OCCOC
Mol. weight [g/mol]:	498.78

Physical Properties

Property code	Value	Unit	Source
gf	-371.12	kJ/mol	Joback Method
hf	-1284.35	kJ/mol	Joback Method
hfus	80.22	kJ/mol	Joback Method
hvap	103.10	kJ/mol	Joback Method
log10ws	-9.19		Crippen Method
logp	8.711		Crippen Method
mcvol	454.310	ml/mol	McGowan Method
pc	617.87	kPa	Joback Method
rinsol	3536.00		NIST Webbook
tb	1060.80	K	Joback Method
tc	1342.66	K	Joback Method
tf	594.41	K	Joback Method
vc	1.782	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1635.72	J/molxK	1060.80	Joback Method
cpg	1659.22	J/molxK	1107.78	Joback Method
cpg	1679.64	J/molxK	1154.75	Joback Method
cpg	1697.10	J/molxK	1201.73	Joback Method
cpg	1711.70	J/molxK	1248.71	Joback Method
cpg	1723.53	J/molxK	1295.68	Joback Method
cpg	1732.70	J/molxK	1342.66	Joback Method
dvisc	0.0001599	Paxs	594.41	Joback Method
dvisc	0.0000735	Paxs	672.14	Joback Method

dvisc	0.0000397	Paxs	749.87	Joback Method
dvisc	0.0000241	Paxs	827.61	Joback Method
dvisc	0.0000159	Paxs	905.34	Joback Method
dvisc	0.0000112	Paxs	983.07	Joback Method
dvisc	0.0000083	Paxs	1060.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355769&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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