

Sebacic acid, hexadecyl 3-methylbutyl ester

Inchi:	InChI=1S/C31H60O4/c1-4-5-6-7-8-9-10-11-12-13-14-17-20-23-27-34-30(32)24-21-18-15
InchiKey:	IRWXJMQXGMKHFP-UHFFFAOYSA-N
Formula:	C31H60O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCCCCCC(=O)OCCC(C)C
Mol. weight [g/mol]:	496.81

Physical Properties

Property code	Value	Unit	Source
gf	-260.14	kJ/mol	Joback Method
hf	-1178.05	kJ/mol	Joback Method
hfus	78.10	kJ/mol	Joback Method
hvap	102.52	kJ/mol	Joback Method
log10ws	-10.28		Crippen Method
logp	9.721		Crippen Method
mvol	462.530	ml/mol	McGowan Method
pc	596.63	kPa	Joback Method
rinpol	3454.00		NIST Webbook
tb	1060.82	K	Joback Method
tc	1339.85	K	Joback Method
tf	568.45	K	Joback Method
vc	1.813	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1671.04	J/molxK	1060.82	Joback Method
cpg	1695.80	J/molxK	1107.32	Joback Method
cpg	1717.77	J/molxK	1153.83	Joback Method
cpg	1737.10	J/molxK	1200.33	Joback Method
cpg	1753.92	J/molxK	1246.84	Joback Method
cpg	1768.37	J/molxK	1293.34	Joback Method
cpg	1780.59	J/molxK	1339.85	Joback Method
dvisc	0.0002323	Paxs	568.45	Joback Method
dvisc	0.0000955	Paxs	650.51	Joback Method

dvisc	0.0000479	Paxs	732.57	Joback Method
dvisc	0.0000276	Paxs	814.64	Joback Method
dvisc	0.0000176	Paxs	896.70	Joback Method
dvisc	0.0000121	Paxs	978.76	Joback Method
dvisc	0.0000088	Paxs	1060.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355380&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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