

Sebacic acid, cis-11-tetradecenyl isoheptyl ester

Inchi:	InChI=1S/C30H56O4/c1-4-5-6-7-8-9-10-11-12-15-18-21-26-33-29(31)24-19-16-13-14-17
InchiKey:	PCWVIMLHSDUBEP-WAYWQWQTS-A-N
Formula:	C30H56O4
SMILES:	CCC=CCCCCCCCCOC(=O)CCCCCCCC(=O)OCCCC(C)C
Mol. weight [g/mol]:	480.76

Physical Properties

Property code	Value	Unit	Source
gf	-188.34	kJ/mol	Joback Method
hf	-1040.19	kJ/mol	Joback Method
hfus	75.71	kJ/mol	Joback Method
hvap	100.26	kJ/mol	Joback Method
log10ws	-9.72		Crippen Method
logp	9.107		Crippen Method
mvol	444.140	ml/mol	McGowan Method
pc	642.22	kPa	Joback Method
rinpol	3358.00		NIST Webbook
tb	1042.10	K	Joback Method
tc	1301.69	K	Joback Method
tf	552.10	K	Joback Method
vc	1.738	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1577.07	J/molxK	1042.10	Joback Method
cpg	1600.54	J/molxK	1085.36	Joback Method
cpg	1621.87	J/molxK	1128.63	Joback Method
cpg	1641.18	J/molxK	1171.89	Joback Method
cpg	1658.60	J/molxK	1215.16	Joback Method
cpg	1674.27	J/molxK	1258.42	Joback Method
cpg	1688.31	J/molxK	1301.69	Joback Method
dvisc	0.0002504	Paxs	552.10	Joback Method
dvisc	0.0001011	Paxs	633.77	Joback Method

dvisc	0.0000502	Paxs	715.43	Joback Method
dvisc	0.0000288	Paxs	797.10	Joback Method
dvisc	0.0000183	Paxs	878.77	Joback Method
dvisc	0.0000126	Paxs	960.43	Joback Method
dvisc	0.0000092	Paxs	1042.10	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356039&Units=SI

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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