Sebacic acid, heptyl tetradecyl ester

Inchi: InChI=1S/C31H60O4/c1-3-5-7-9-10-11-12-13-14-17-21-25-29-35-31(33)27-23-19-16-15-
InchiKey: VKMLCWUHDOXEDY-UHFFFAOYSA-N
Formula: C31H60O4
SMILES: CCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCCCCCC
Mol. weight [g/mol]: 496.81

Physical Properties

Property code	Value	Unit	Source
gf	-257.70	kJ/mol	Joback Method
hf	-1172.77	kJ/mol	Joback Method
hfus	81.62	kJ/mol	Joback Method
hvap	102.91	kJ/mol	Joback Method
log10ws	-10.52		Crippen Method
logp	9.865		Crippen Method
mcvol	462.530	ml/mol	McGowan Method
pc	594.30	kPa	Joback Method
rinpol	3546.00		NIST Webbook
tb	1061.26	K	Joback Method
tc	1344.42	K	Joback Method
tf	583.45	K	Joback Method
vc	1.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1670.89	J/mol×K	1061.26	Joback Method
cpg	1769.95	J/mol×K	1297.22	Joback Method
cpg	1755.25	J/mol×K	1250.03	Joback Method
cpg	1738.13	J/mol×K	1202.84	Joback Method
cpg	1718.46	J/mol×K	1155.65	Joback Method
cpg	1696.10	J/mol×K	1108.45	Joback Method
cpg	1782.40	J/mol×K	1344.42	Joback Method
dvisc	0.0000097	Pa×s	1061.26	Joback Method
dvisc	0.0000132	Pa×s	981.62	Joback Method

dvisc	0.0000188	Pa×s	901.99	Joback Method
dvisc	0.0000288	Pa×s	822.36	Joback Method
dvisc	0.0000484	Pa×s	742.72	Joback Method
dvisc	0.0000918	Pa×s	663.08	Joback Method
dvisc	0.0002077	Pa×s	583.45	Joback Method

Sources

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=U354311&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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