Sebacic acid, heptadecyl isobutyl ester

Inchi: InChI=1S/C31H60O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-18-21-24-27-34-30(32)25-22-19
InchiKey: XZANTWRLLXJWNO-UHFFFAOYSA-N
Formula: C31H60O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC(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
mcvol	462.530	ml/mol	McGowan Method
pc	596.63	kPa	Joback Method
rinpol	3512.00		NIST Webbook
rinpol	3512.00		NIST Webbook
tb	1060.82	K	Joback Method
tc	1339.85	K	Joback Method
tf	568.45	K	Joback Method
vc	1.813	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1671.04	J/mol×K	1060.82	Joback Method
cpg	1695.80	J/mol×K	1107.32	Joback Method
cpg	1717.77	J/mol×K	1153.83	Joback Method
cpg	1737.10	J/mol×K	1200.33	Joback Method
cpg	1753.92	J/mol×K	1246.84	Joback Method
cpg	1768.37	J/mol×K	1293.34	Joback Method
cpg	1780.59	J/mol×K	1339.85	Joback Method
dvisc	0.0002323	Pa×s	568.45	Joback Method

dvisc	0.0000955	Pa×s	650.51	Joback Method
dvisc	0.0000479	Pa×s	732.57	Joback Method
dvisc	0.0000276	Pa×s	814.64	Joback Method
dvisc	0.0000176	Pa×s	896.70	Joback Method
dvisc	0.0000121	Pa×s	978.76	Joback Method
dvisc	0.0000088	Pa×s	1060.82	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=U354229&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