Sebacic acid, hexadecyl oct-3-yl ester

Inchi: InChI=1S/C34H66O4/c1-4-7-9-10-11-12-13-14-15-16-17-20-23-27-31-37-33(35)29-25-21
InchiKey: XPEDMVIWNHHRTA-UHFFFAOYSA-N
Formula: C34H66O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OC(CC)CCCCC
Mol. weight [g/mol]: 538.89

Physical Properties

Property code	Value	Unit	Source
gf	-234.88	kJ/mol	Joback Method
hf	-1239.97	kJ/mol	Joback Method
hfus	85.87	kJ/mol	Joback Method
hvap	109.20	kJ/mol	Joback Method
log10ws	-11.89		Crippen Method
logp	11.034		Crippen Method
mcvol	504.800	ml/mol	McGowan Method
pc	520.78	kPa	Joback Method
rinpol	3365.00		NIST Webbook
rinpol	3365.00		NIST Webbook
tb	1129.46	K	Joback Method
tc	1465.72	K	Joback Method
tf	602.26	K	Joback Method
vc	1.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1869.01	J/mol×K	1129.46	Joback Method
cpg	1896.47	J/mol×K	1185.50	Joback Method
cpg	1920.00	J/mol×K	1241.55	Joback Method
cpg	1939.87	J/mol×K	1297.59	Joback Method
cpg	1956.37	J/mol×K	1353.64	Joback Method
cpg	1969.78	J/mol×K	1409.68	Joback Method
cpg	1980.37	J/mol×K	1465.72	Joback Method
dvisc	0.0001493	Pa×s	602.26	Joback Method

dvisc	0.0000603	Pa×s	690.13	Joback Method
dvisc	0.0000299	Pa×s	777.99	Joback Method
dvisc	0.0000171	Pa×s	865.86	Joback Method
dvisc	0.0000108	Pa×s	953.73	Joback Method
dvisc	0.0000074	Pa×s	1041.59	Joback Method
dvisc	0.0000054	Pa×s	1129.46	Joback Method

Sources

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=U416840&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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