Diethylmalonic acid, octadecyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C33H64O4/c1-8-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-36-30(34)
InchiKey: HZJKCUQCXRQNBD-UHFFFAOYSA-N
Formula: C33H64O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]: 524.86

Physical Properties

Property code	Value	Unit	Source
gf	-237.62	kJ/mol	Joback Method
hf	-1236.83	kJ/mol	Joback Method
hfus	68.45	kJ/mol	Joback Method
hvap	104.38	kJ/mol	Joback Method
log10ws	-10.64		Crippen Method
logp	10.213		Crippen Method
mcvol	490.710	ml/mol	McGowan Method
pc	554.15	kPa	Joback Method
rinpol	3235.00		NIST Webbook
tb	1100.12	K	Joback Method
tc	1386.33	K	Joback Method
tf	595.83	K	Joback Method
vc	1.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1802.91	J/mol×K	1100.12	Joback Method
cpg	1912.13	J/mol×K	1338.63	Joback Method
cpg	1893.73	J/mol×K	1290.92	Joback Method
cpg	1873.86	J/mol×K	1243.22	Joback Method
cpg	1852.27	J/mol×K	1195.52	Joback Method
cpg	1828.71	J/mol×K	1147.82	Joback Method
cpg	1929.34	J/mol×K	1386.33	Joback Method
dvisc	0.0000035	Pa×s	1100.12	Joback Method
dvisc	0.0000049	Pa×s	1016.07	Joback Method

dvisc	0.0000074	Pa×s	932.02	Joback Method
dvisc	0.0000122	Pa×s	847.97	Joback Method
dvisc	0.0000224	Pa×s	763.93	Joback Method
dvisc	0.0000478	Pa×s	679.88	Joback Method
dvisc	0.0001261	Pa×s	595.83	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=U369490&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