Diethylmalonic acid, 3,7-dimethyloctyl heptadecyl ester

Inchi: InChI=1S/C34H66O4/c1-7-10-11-12-13-14-15-16-17-18-19-20-21-22-23-28-37-32(35)34(
InchiKey: XNTPIYMDLMXXQD-UHFFFAOYSA-N
Formula: C34H66O4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCC(C)CCCC(C)C
Mol. weight [g/mol]: 538.89

Physical Properties

Property code	Value	Unit	Source
gf	-234.48	kJ/mol	Joback Method
hf	-1254.00	kJ/mol	Joback Method
hfus	74.93	kJ/mol	Joback Method
hvap	107.52	kJ/mol	Joback Method
log10ws	-11.05		Crippen Method
logp	10.603		Crippen Method
mcvol	504.800	ml/mol	McGowan Method
pc	527.26	kPa	Joback Method
rinpol	3317.00		NIST Webbook
tb	1125.79	K	Joback Method
tc	1439.17	K	Joback Method
tf	589.68	K	Joback Method
vc	1.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1869.33	J/mol×K	1125.79	Joback Method
cpg	1895.97	J/mol×K	1178.02	Joback Method
cpg	1919.59	J/mol×K	1230.25	Joback Method
cpg	1940.46	J/mol×K	1282.48	Joback Method
cpg	1958.88	J/mol×K	1334.71	Joback Method
cpg	1975.14	J/mol×K	1386.94	Joback Method
cpg	1989.52	J/mol×K	1439.17	Joback Method
dvisc	0.0001429	Pa×s	589.68	Joback Method
dvisc	0.0000516	Pa×s	679.03	Joback Method

dvisc	0.0000236	Pa×s	768.38	Joback Method
dvisc	0.0000127	Pa×s	857.73	Joback Method
dvisc	0.0000077	Pa×s	947.09	Joback Method
dvisc	0.0000051	Pa×s	1036.44	Joback Method
dvisc	0.0000036	Pa×s	1125.79	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U369415&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