Dimethylmalonic acid, heptadecyl undecyl ester

Inchi: InChI=1S/C33H64O4/c1-5-7-9-11-13-15-16-17-18-19-20-22-24-26-28-30-37-32(35)33(3,4

InchiKey: DRUUAJQMWAVNBG-UHFFFAOYSA-N

Formula: C33H64O4

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCCCCCCCCCCC

Mol. weight [g/mol]: 524.86

Physical Properties

Property code	Value	Unit	Source
gf	-238.02	kJ/mol	Joback Method
hf	-1222.80	kJ/mol	Joback Method
hfus	79.39	kJ/mol	Joback Method
hvap	106.07	kJ/mol	Joback Method
log10ws	-11.12		Crippen Method
logp	10.501		Crippen Method
mcvol	490.710	ml/mol	McGowan Method
pc	547.18	kPa	Joback Method
rinpol	3388.00		NIST Webbook
rinpol	3388.00		NIST Webbook
tb	1103.79	K	Joback Method
tc	1408.20	K	Joback Method
tf	608.41	K	Joback Method
vc	1.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1802.89	J/mol×K	1103.79	Joback Method
cpg	1910.23	J/mol×K	1357.47	Joback Method
cpg	1893.46	J/mol×K	1306.73	Joback Method
cpg	1874.60	J/mol×K	1256.00	Joback Method
cpg	1853.39	J/mol×K	1205.26	Joback Method
cpg	1829.57	J/mol×K	1154.53	Joback Method
cpg	1925.16	J/mol×K	1408.20	Joback Method
dvisc	0.0000052	Pa×s	1103.79	Joback Method

dvisc	0.0000071	Pa×s	1021.23	Joback Method
dvisc	0.0000104	Pa×s	938.66	Joback Method
dvisc	0.0000164	Pa×s	856.10	Joback Method
dvisc	0.0000283	Pa×s	773.54	Joback Method
dvisc	0.0000558	Pa×s	690.97	Joback Method
dvisc	0.0001323	Pa×s	608.41	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=U361786&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