

Dimethylmalonic acid, ditetradecyl ester

Inchi: InChI=1S/C33H64O4/c1-5-7-9-11-13-15-17-19-21-23-25-27-29-36-31(34)33(3,4)32(35)3
InchiKey: MVGRFICXOGUODJ-UHFFFAOYSA-N
Formula: C33H64O4
SMILES: CCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCCCCCCCCCCCCC
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	3391.00		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/molxK	1103.79	Joback Method
cpg	1910.23	J/molxK	1357.47	Joback Method
cpg	1893.46	J/molxK	1306.73	Joback Method
cpg	1874.60	J/molxK	1256.00	Joback Method
cpg	1853.39	J/molxK	1205.26	Joback Method
cpg	1829.57	J/molxK	1154.53	Joback Method
cpg	1925.16	J/molxK	1408.20	Joback Method
dvisc	0.0000052	Paxs	1103.79	Joback Method
dvisc	0.0000071	Paxs	1021.23	Joback Method

dvisc	0.0000104	Paxs	938.66	Joback Method
dvisc	0.0000164	Paxs	856.10	Joback Method
dvisc	0.0000283	Paxs	773.54	Joback Method
dvisc	0.0000558	Paxs	690.97	Joback Method
dvisc	0.0001323	Paxs	608.41	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=U361768&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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

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