Dimethylmalonic acid, tetradecyl undecyl ester

Inchi: InChI=1S/C30H58O4/c1-5-7-9-11-13-15-16-17-19-21-23-25-27-34-29(32)30(3,4)28(31)3

InchiKey: CJRKDJQLXCNBEA-UHFFFAOYSA-N

Formula: C30H58O4

SMILES: CCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCCCCCCCCCCCC

Mol. weight [g/mol]: 482.78

Physical Properties

Property code	Value	Unit	Source
gf	-263.28	kJ/mol	Joback Method
hf	-1160.88	kJ/mol	Joback Method
hfus	71.62	kJ/mol	Joback Method
hvap	99.39	kJ/mol	Joback Method
log10ws	-9.86		Crippen Method
logp	9.331		Crippen Method
mcvol	448.440	ml/mol	McGowan Method
pc	629.08	kPa	Joback Method
rinpol	3088.00		NIST Webbook
tb	1035.15	K	Joback Method
tc	1291.99	K	Joback Method
tf	574.60	K	Joback Method
vc	1.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1604.78	J/mol×K	1035.15	Joback Method
cpg	1703.68	J/mol×K	1249.18	Joback Method
cpg	1687.63	J/mol×K	1206.38	Joback Method
cpg	1669.84	J/mol×K	1163.57	Joback Method
cpg	1650.20	J/mol×K	1120.76	Joback Method
cpg	1628.56	J/mol×K	1077.96	Joback Method
cpg	1718.15	J/mol×K	1291.99	Joback Method
dvisc	0.0000086	Pa×s	1035.15	Joback Method
dvisc	0.0000118	Pa×s	958.39	Joback Method

dvisc	0.0000171	Pa×s	881.63	Joback Method
dvisc	0.0000267	Pa×s	804.88	Joback Method
dvisc	0.0000457	Pa×s	728.12	Joback Method
dvisc	0.0000890	Pa×s	651.36	Joback Method
dvisc	0.0002068	Pa×s	574.60	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=U361765&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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