Dimethylmalonic acid, heptyl octadecyl ester

Inchi: InChI=1S/C30H58O4/c1-5-7-9-11-12-13-14-15-16-17-18-19-20-21-23-25-27-34-29(32)30
InchiKey: NCTIMTRLWQZENJ-UHFFFAOYSA-N
Formula: C30H58O4
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCCCCCCC
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	3111.00		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	1628.56	J/mol×K	1077.96	Joback Method
cpg	1650.20	J/mol×K	1120.76	Joback Method
cpg	1669.84	J/mol×K	1163.57	Joback Method
cpg	1687.63	J/mol×K	1206.38	Joback Method
cpg	1703.68	J/mol×K	1249.18	Joback Method
cpg	1718.15	J/mol×K	1291.99	Joback Method
dvisc	0.0002068	Pa×s	574.60	Joback Method
dvisc	0.0000890	Pa×s	651.36	Joback Method

dvisc	0.0000457	Pa×s	728.12	Joback Method
dvisc	0.0000267	Pa×s	804.88	Joback Method
dvisc	0.0000171	Pa×s	881.63	Joback Method
dvisc	0.0000118	Pa×s	958.39	Joback Method
dvisc	0.0000086	Pa×s	1035.15	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361909&Units=SI

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

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