Dimethylmalonic acid, 3-methylbutyl octadecyl ester

Inchi: InChI=1S/C28H54O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-23-31-26(29)28(
InchiKey: PFILMFPPWDHVOV-UHFFFAOYSA-N
Formula: C28H54O4
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCCC(C)C
Mol. weight [g/mol]: 454.73

Physical Properties

Property code	Value	Unit	Source
gf	-282.56	kJ/mol	Joback Method
hf	-1124.88	kJ/mol	Joback Method
hfus	62.91	kJ/mol	Joback Method
hvap	94.55	kJ/mol	Joback Method
log10ws	-8.78		Crippen Method
logp	8.407		Crippen Method
mcvol	420.260	ml/mol	McGowan Method
pc	697.28	kPa	Joback Method
rinpol	2877.00		NIST Webbook
rinpol	2877.00		NIST Webbook
tb	988.95	K	Joback Method
tc	1220.27	K	Joback Method
tf	537.06	K	Joback Method
vc	1.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1474.43	J/mol×K	988.95	Joback Method
cpg	1496.42	J/mol×K	1027.50	Joback Method
cpg	1516.64	J/mol×K	1066.06	Joback Method
cpg	1535.17	J/mol×K	1104.61	Joback Method
cpg	1552.12	J/mol×K	1143.16	Joback Method
cpg	1567.57	J/mol×K	1181.71	Joback Method
cpg	1581.62	J/mol×K	1220.27	Joback Method
dvisc	0.0003161	Pa×s	537.06	Joback Method

dvisc	0.0001276	Pa×s	612.38	Joback Method
dvisc	0.0000628	Pa×s	687.69	Joback Method
dvisc	0.0000356	Pa×s	763.00	Joback Method
dvisc	0.0000223	Pa×s	838.32	Joback Method
dvisc	0.0000151	Pa×s	913.63	Joback Method
dvisc	0.0000109	Pa×s	988.95	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=U361605&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