Dimethylmalonic acid, neopentyl pentyl ester

Inchi: InChI=1S/C15H28O4/c1-7-8-9-10-18-12(16)15(5,6)13(17)19-11-14(2,3)4/h7-11H2,1-6H3
InchiKey: ZVKYKSQPTRELSZ-UHFFFAOYSA-N
Formula: C15H28O4
SMILES: CCCCCOC(=O)C(C)(C)C(=O)OCC(C)(C)C
Mol. weight [g/mol]: 272.38

Physical Properties

Property code	Value	Unit	Source
gf	-386.74	kJ/mol	Joback Method
hf	-860.03	kJ/mol	Joback Method
hfus	25.35	kJ/mol	Joback Method
hvap	64.70	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.335		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
pc	1564.75	kPa	Joback Method
rinpol	1547.00		NIST Webbook
tb	688.72	K	Joback Method
tc	878.18	K	Joback Method
tf	407.97	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.02	J/mol×K	688.72	Joback Method
cpg	757.49	J/mol×K	846.60	Joback Method
cpg	744.17	J/mol×K	815.02	Joback Method
cpg	730.00	J/mol×K	783.45	Joback Method
cpg	714.94	J/mol×K	751.87	Joback Method
cpg	698.96	J/mol×K	720.30	Joback Method
cpg	769.98	J/mol×K	878.18	Joback Method
dvisc	0.0000754	Pa×s	688.72	Joback Method
dvisc	0.0001030	Pa×s	641.93	Joback Method

dvisc	0.0001476	Pa×s	595.14	Joback Method
dvisc	0.0002250	Pa×s	548.35	Joback Method
dvisc	0.0003711	Pa×s	501.55	Joback Method
dvisc	0.0006784	Pa×s	454.76	Joback Method
dvisc	0.0014241	Pa×s	407.97	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=U361745&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