Dimethylmalonic acid, dineopentyl ester

Inchi: InChI=1S/C15H28O4/c1-13(2,3)9-18-11(16)15(7,8)12(17)19-10-14(4,5)6/h9-10H2,1-8H3
InchiKey: KTPGOWDCUARQOF-UHFFFAOYSA-N
Formula: C15H28O4
SMILES: CC(C)(C)COC(=O)C(C)(C)C(=O)OCC(C)(C)C
Mol. weight [g/mol]: 272.38

Physical Properties

Property code	Value	Unit	Source
gf	-383.90	kJ/mol	Joback Method
hf	-868.78	kJ/mol	Joback Method
hfus	17.94	kJ/mol	Joback Method
hvap	63.41	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	3.191		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
pc	1588.54	kPa	Joback Method
rinpol	1453.00		NIST Webbook
tb	685.49	K	Joback Method
tc	883.45	K	Joback Method
tf	410.39	K	Joback Method
vc	0.890	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.46	J/mol×K	685.49	Joback Method
cpg	701.94	J/mol×K	718.48	Joback Method
cpg	718.33	J/mol×K	751.48	Joback Method
cpg	733.70	J/mol×K	784.47	Joback Method
cpg	748.10	J/mol×K	817.47	Joback Method
cpg	761.57	J/mol×K	850.46	Joback Method
cpg	774.19	J/mol×K	883.45	Joback Method
dvisc	0.0014379	Pa×s	410.39	Joback Method
dvisc	0.0006598	Pa×s	456.24	Joback Method

dvisc	0.0003491	Pa×s	502.09	Joback Method
dvisc	0.0002054	Pa×s	547.94	Joback Method
dvisc	0.0001312	Pa×s	593.79	Joback Method
dvisc	0.0000894	Pa×s	639.64	Joback Method
dvisc	0.0000641	Pa×s	685.49	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=U361759&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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