Dimethylmalonic acid, dodecyl neopentyl ester

Inchi: InChI=1S/C22H42O4/c1-7-8-9-10-11-12-13-14-15-16-17-25-19(23)22(5,6)20(24)26-18-2
InchiKey: QEQAKCBHYUVDKH-UHFFFAOYSA-N
Formula: C22H42O4
SMILES: CCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCC(C)(C)C
Mol. weight [g/mol]: 370.57

Physical Properties

Property code	Value	Unit	Source
gf	-327.80	kJ/mol	Joback Method
hf	-1004.51	kJ/mol	Joback Method
hfus	43.48	kJ/mol	Joback Method
hvap	80.29	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	6.066		Crippen Method
mcvol	335.720	ml/mol	McGowan Method
pc	976.56	kPa	Joback Method
rinpol	2234.00		NIST Webbook
tb	848.88	K	Joback Method
tc	1042.22	K	Joback Method
tf	486.86	K	Joback Method
vc	1.294	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.11	J/mol×K	848.88	Joback Method
cpg	1112.02	J/mol×K	881.10	Joback Method
cpg	1129.79	J/mol×K	913.33	Joback Method
cpg	1146.46	J/mol×K	945.55	Joback Method
cpg	1162.10	J/mol×K	977.77	Joback Method
cpg	1176.74	J/mol×K	1010.00	Joback Method
cpg	1190.46	J/mol×K	1042.22	Joback Method
dvisc	0.0005794	Pa×s	486.86	Joback Method
dvisc	0.0002564	Pa×s	547.20	Joback Method

dvisc	0.0001334	Pa×s	607.53	Joback Method
dvisc	0.0000781	Pa×s	667.87	Joback Method
dvisc	0.0000500	Pa×s	728.21	Joback Method
dvisc	0.0000342	Pa×s	788.54	Joback Method
dvisc	0.0000248	Pa×s	848.88	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=U361752&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