Dimethylmalonic acid, isobutyl neopentyl ester

Inchi: InChI=1S/C14H26O4/c1-10(2)8-17-11(15)14(6,7)12(16)18-9-13(3,4)5/h10H,8-9H2,1-7H3

InchiKey: LFRIQNIYNUVMTE-UHFFFAOYSA-N

Formula: C14H26O4

SMILES: CC(C)COC(=O)C(C)(C)C(=O)OCC(C)(C)C

Mol. weight [g/mol]: 258.35

Physical Properties

Property code	Value	Unit	Source
gf	-397.60	kJ/mol	Joback Method
hf	-844.67	kJ/mol	Joback Method
hfus	19.24	kJ/mol	Joback Method
hvap	62.09	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.801		Crippen Method
mcvol	223.000	ml/mol	McGowan Method
pc	1701.90	kPa	Joback Method
rinpol	1416.00		NIST Webbook
rinpol	1416.00		NIST Webbook
tb	665.40	K	Joback Method
tc	859.55	K	Joback Method
tf	381.70	K	Joback Method
vc	0.840	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.85	J/mol×K	665.40	Joback Method
cpg	644.76	J/mol×K	697.76	Joback Method
cpg	660.69	J/mol×K	730.12	Joback Method
cpg	675.68	J/mol×K	762.48	Joback Method
cpg	689.75	J/mol×K	794.84	Joback Method
cpg	702.96	J/mol×K	827.19	Joback Method
cpg	715.32	J/mol×K	859.55	Joback Method
dvisc	0.0020424	Pa×s	381.70	Joback Method

dvisc	0.0008881	Pa×s	428.98	Joback Method
dvisc	0.0004556	Pa×s	476.27	Joback Method
dvisc	0.0002637	Pa×s	523.55	Joback Method
dvisc	0.0001671	Pa×s	570.83	Joback Method
dvisc	0.0001135	Pa×s	618.12	Joback Method
dvisc	0.0000815	Pa×s	665.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361744&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