Dimethylmalonic acid, isobutyl 2-pentyl ester

Inchi: InChI=1S/C14H26O4/c1-7-8-11(4)18-13(16)14(5,6)12(15)17-9-10(2)3/h10-11H,7-9H2,1-
InchiKey: OBGWFDUVCOJBLM-UHFFFAOYSA-N
Formula: C14H26O4
SMILES: CCCC(C)OC(=O)C(C)(C)C(=O)OCC(C)C
Mol. weight [g/mol]: 258.35

Physical Properties

Property code	Value	Unit	Source
gf	-402.88	kJ/mol	Joback Method
hf	-841.20	kJ/mol	Joback Method
hfus	23.13	kJ/mol	Joback Method
hvap	63.00	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.944		Crippen Method
mcvol	223.000	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
rinpol	1472.00		NIST Webbook
rinpol	1472.00		NIST Webbook
tb	668.19	K	Joback Method
tc	856.76	K	Joback Method
tf	364.28	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.68	J/mol×K	668.19	Joback Method
cpg	642.32	J/mol×K	699.62	Joback Method
cpg	658.07	J/mol×K	731.05	Joback Method
cpg	672.95	J/mol×K	762.47	Joback Method
cpg	686.98	J/mol×K	793.90	Joback Method
cpg	700.18	J/mol×K	825.33	Joback Method
cpg	712.56	J/mol×K	856.76	Joback Method
dvisc	0.0025067	Pa×s	364.28	Joback Method

dvisc	0.0010206	Pa×s	414.93	Joback Method
dvisc	0.0005053	Pa×s	465.58	Joback Method
dvisc	0.0002872	Pa×s	516.24	Joback Method
dvisc	0.0001805	Pa×s	566.89	Joback Method
dvisc	0.0001225	Pa×s	617.54	Joback Method
dvisc	0.0000881	Pa×s	668.19	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=U361580&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

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