Dimethylmalonic acid, hexyl isobutyl ester

Inchi: InChI=1S/C15H28O4/c1-6-7-8-9-10-18-13(16)15(4,5)14(17)19-11-12(2)3/h12H,6-11H2,1
InchiKey: KHMQSUWTIUSIRV-UHFFFAOYSA-N
Formula: C15H28O4
SMILES: CCCCCCOC(=O)C(C)(C)C(=O)OCC(C)C
Mol. weight [g/mol]: 272.38

Physical Properties

Property code	Value	Unit	Source
gf	-392.02	kJ/mol	Joback Method
hf	-856.56	kJ/mol	Joback Method
hfus	29.24	kJ/mol	Joback Method
hvap	65.61	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.335		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
pc	1551.22	kPa	Joback Method
rinpol	1607.00		NIST Webbook
rinpol	1607.00		NIST Webbook
tb	691.51	K	Joback Method
tc	876.12	K	Joback Method
tf	390.55	K	Joback Method
vc	0.906	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.11	J/mol×K	691.51	Joback Method
cpg	696.84	J/mol×K	722.28	Joback Method
cpg	712.70	J/mol×K	753.05	Joback Method
cpg	727.68	J/mol×K	783.82	Joback Method
cpg	741.83	J/mol×K	814.59	Joback Method
cpg	755.14	J/mol×K	845.35	Joback Method
cpg	767.65	J/mol×K	876.12	Joback Method
dvisc	0.0017437	Pa×s	390.55	Joback Method

dvisc	0.0007852	Pa×s	440.71	Joback Method
dvisc	0.0004162	Pa×s	490.87	Joback Method
dvisc	0.0002481	Pa×s	541.03	Joback Method
dvisc	0.0001615	Pa×s	591.19	Joback Method
dvisc	0.0001124	Pa×s	641.35	Joback Method
dvisc	0.0000825	Pa×s	691.51	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=U361654&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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