Dimethylmalonic acid, isobutyl 2-methylpent-3-yl ester

Inchi: InChI=1S/C15H28O4/c1-8-12(11(4)5)19-14(17)15(6,7)13(16)18-9-10(2)3/h10-12H,8-9H2

InchiKey: QCQVUQSDIOUXNH-UHFFFAOYSA-N

Formula: C15H28O4

SMILES: CCC(OC(=O)C(C)(C)C(=O)OCC(C)C)C(C)C

Mol. weight [g/mol]: 272.38

Physical Properties

Property code	Value	Unit	Source
gf	-396.90	kJ/mol	Joback Method
hf	-867.12	kJ/mol	Joback Method
hfus	22.20	kJ/mol	Joback Method
hvap	64.84	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	3.190		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
pc	1570.96	kPa	Joback Method
rinpol	1556.00		NIST Webbook
rinpol	1556.00		NIST Webbook
tb	690.63	K	Joback Method
tc	880.65	K	Joback Method
tf	360.55	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.05	J/mol×K	690.63	Joback Method
cpg	698.33	J/mol×K	722.30	Joback Method
cpg	714.65	J/mol×K	753.97	Joback Method
cpg	730.05	J/mol×K	785.64	Joback Method
cpg	744.53	J/mol×K	817.31	Joback Method
cpg	758.12	J/mol×K	848.98	Joback Method
cpg	770.84	J/mol×K	880.65	Joback Method
dvisc	0.0029478	Pa×s	360.55	Joback Method

dvisc	0.0010492	Pa×s	415.56	Joback Method
dvisc	0.0004755	Pa×s	470.58	Joback Method
dvisc	0.0002543	Pa×s	525.59	Joback Method
dvisc	0.0001531	Pa×s	580.60	Joback Method
dvisc	0.0001007	Pa×s	635.62	Joback Method
dvisc	0.0000708	Pa×s	690.63	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361789&Units=SI

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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