

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,7-9H2,1-4H3
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
mvol	223.000	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
rinpol	1472.00		NIST Webbook
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tb	668.19	K	Joback Method
tc	856.76	K	Joback Method
tf	364.28	K	Joback Method
vc	0.845	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.68	J/molxK	668.19	Joback Method
cpg	700.18	J/molxK	825.33	Joback Method
cpg	686.98	J/molxK	793.90	Joback Method
cpg	672.95	J/molxK	762.47	Joback Method
cpg	658.07	J/molxK	731.05	Joback Method
cpg	642.32	J/molxK	699.62	Joback Method
cpg	712.56	J/molxK	856.76	Joback Method
dvisc	0.0000881	Paxs	668.19	Joback Method

dvisc	0.0001225	Paxs	617.54	Joback Method
dvisc	0.0001805	Paxs	566.89	Joback Method
dvisc	0.0002872	Paxs	516.24	Joback Method
dvisc	0.0005053	Paxs	465.58	Joback Method
dvisc	0.0010206	Paxs	414.93	Joback Method
dvisc	0.0025067	Paxs	364.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361580&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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