

Dimethylmalonic acid, monochloride, isobutyl ester

Inchi:	InChI=1S/C9H15ClO3/c1-6(2)5-13-8(12)9(3,4)7(10)11/h6H,5H2,1-4H3
InchiKey:	GOYWSOYAZVNGHL-UHFFFAOYSA-N
Formula:	C9H15ClO3
SMILES:	CC(C)COC(=O)C(C)(C)C(=O)Cl
Mol. weight [g/mol]:	206.67

Physical Properties

Property code	Value	Unit	Source
gf	-349.47	kJ/mol	Joback Method
hf	-616.24	kJ/mol	Joback Method
hfus	16.71	kJ/mol	Joback Method
hvap	54.23	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	1.977		Crippen Method
mcvol	158.920	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
rinpol	1145.00		NIST Webbook
tb	569.24	K	Joback Method
tc	771.37	K	Joback Method
tf	330.62	K	Joback Method
vc	0.602	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.47	J/molxK	569.24	Joback Method
cpg	387.39	J/molxK	602.93	Joback Method
cpg	399.58	J/molxK	636.62	Joback Method
cpg	411.05	J/molxK	670.31	Joback Method
cpg	421.83	J/molxK	703.99	Joback Method
cpg	431.94	J/molxK	737.68	Joback Method
cpg	441.41	J/molxK	771.37	Joback Method
dvisc	0.0035847	Paxs	330.62	Joback Method
dvisc	0.0017420	Paxs	370.39	Joback Method

dvisc	0.0009737	Paxs	410.16	Joback Method
dvisc	0.0006032	Paxs	449.93	Joback Method
dvisc	0.0004039	Paxs	489.70	Joback Method
dvisc	0.0002872	Paxs	529.47	Joback Method
dvisc	0.0002142	Paxs	569.24	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361667&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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