

Dimethylmalonic acid, monochloride, hexyl ester

Inchi:	InChI=1S/C11H19ClO3/c1-4-5-6-7-8-15-10(14)11(2,3)9(12)13/h4-8H2,1-3H3
InchiKey:	XGKCWKZFGZFKAR-UHFFFAOYSA-N
Formula:	C11H19ClO3
SMILES:	CCCCCOC(=O)C(C)(C)C(=O)Cl
Mol. weight [g/mol]:	234.72

Physical Properties

Property code	Value	Unit	Source
gf	-330.19	kJ/mol	Joback Method
hf	-652.24	kJ/mol	Joback Method
hfus	25.41	kJ/mol	Joback Method
hvap	59.07	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.901		Crippen Method
mcvol	187.100	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
rinpol	1396.00		NIST Webbook
rinpol	1396.00		NIST Webbook
tb	615.44	K	Joback Method
tc	808.46	K	Joback Method
tf	368.16	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.83	J/molxK	615.44	Joback Method
cpg	484.79	J/molxK	647.61	Joback Method
cpg	497.98	J/molxK	679.78	Joback Method
cpg	510.44	J/molxK	711.95	Joback Method
cpg	522.18	J/molxK	744.12	Joback Method
cpg	533.23	J/molxK	776.29	Joback Method
cpg	543.62	J/molxK	808.46	Joback Method
dvisc	0.0023713	Paxs	368.16	Joback Method

dvisc	0.0012395	Paxs	409.37	Joback Method
dvisc	0.0007295	Paxs	450.59	Joback Method
dvisc	0.0004692	Paxs	491.80	Joback Method
dvisc	0.0003231	Paxs	533.01	Joback Method
dvisc	0.0002348	Paxs	574.23	Joback Method
dvisc	0.0001780	Paxs	615.44	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=U361700&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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