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: CCCCCCOC(=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/mol×K	615.44	Joback Method
cpg	484.79	J/mol×K	647.61	Joback Method
cpg	497.98	J/mol×K	679.78	Joback Method
cpg	510.44	J/mol×K	711.95	Joback Method
cpg	522.18	J/mol×K	744.12	Joback Method
cpg	533.23	J/mol×K	776.29	Joback Method
cpg	543.62	J/mol×K	808.46	Joback Method
dvisc	0.0023713	Pa×s	368.16	Joback Method

dvisc	0.0012395	Pa×s	409.37	Joback Method
dvisc	0.0007295	Pa×s	450.59	Joback Method
dvisc	0.0004692	Pa×s	491.80	Joback Method
dvisc	0.0003231	Pa×s	533.01	Joback Method
dvisc	0.0002348	Pa×s	574.23	Joback Method
dvisc	0.0001780	Pa×s	615.44	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=U361700&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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