

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

Inchi:	InChI=1S/C11H19ClO3/c1-6-8(7(2)3)15-10(14)11(4,5)9(12)13/h7-8H,6H2,1-5H3
InchiKey:	FPLGPYWSBFFAOD-UHFFFAOYSA-N
Formula:	C11H19ClO3
SMILES:	CCC(OC(=O)C(C)(C)C(=O)Cl)C(C)C
Mol. weight [g/mol]:	234.72

Physical Properties

Property code	Value	Unit	Source
gf	-335.07	kJ/mol	Joback Method
hf	-662.80	kJ/mol	Joback Method
hfus	18.37	kJ/mol	Joback Method
hvap	58.30	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.756		Crippen Method
mcvol	187.100	ml/mol	McGowan Method
pc	2129.52	kPa	Joback Method
rinsol	1341.00		NIST Webbook
tb	614.56	K	Joback Method
tc	814.90	K	Joback Method
tf	338.16	K	Joback Method
vc	0.708	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.70	J/molxK	614.56	Joback Method
cpg	486.28	J/molxK	647.95	Joback Method
cpg	500.02	J/molxK	681.34	Joback Method
cpg	512.95	J/molxK	714.73	Joback Method
cpg	525.08	J/molxK	748.12	Joback Method
cpg	536.46	J/molxK	781.51	Joback Method
cpg	547.11	J/molxK	814.90	Joback Method
dvisc	0.0040182	Paxs	338.16	Joback Method
dvisc	0.0016868	Paxs	384.23	Joback Method

dvisc	0.0008527	Paxs	430.29	Joback Method
dvisc	0.0004919	Paxs	476.36	Joback Method
dvisc	0.0003126	Paxs	522.43	Joback Method
dvisc	0.0002139	Paxs	568.49	Joback Method
dvisc	0.0001549	Paxs	614.56	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=U361805&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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