

Malonic acid, 2-chloropropyl propyl ester

Inchi:	InChI=1S/C9H15ClO4/c1-3-4-13-8(11)5-9(12)14-6-7(2)10/h7H,3-6H2,1-2H3
InchiKey:	IQLRLUZXLPNYMG-UHFFFAOYSA-N
Formula:	C9H15ClO4
SMILES:	CCCOC(=O)CC(=O)OCC(C)Cl
Mol. weight [g/mol]:	222.67

Physical Properties

Property code	Value	Unit	Source
gf	-457.31	kJ/mol	Joback Method
hf	-739.71	kJ/mol	Joback Method
hfus	25.31	kJ/mol	Joback Method
hvap	57.94	kJ/mol	Joback Method
log10ws	-1.58		Crippen Method
logp	1.500		Crippen Method
mcvol	164.790	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method
rinsol	1424.00		NIST Webbook
tb	594.89	K	Joback Method
tc	784.66	K	Joback Method
tf	350.43	K	Joback Method
vc	0.630	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.30	J/molxK	594.89	Joback Method
cpg	407.39	J/molxK	626.52	Joback Method
cpg	418.93	J/molxK	658.15	Joback Method
cpg	429.91	J/molxK	689.78	Joback Method
cpg	440.35	J/molxK	721.41	Joback Method
cpg	450.22	J/molxK	753.04	Joback Method
cpg	459.52	J/molxK	784.66	Joback Method
dvisc	0.0021843	Paxs	350.43	Joback Method
dvisc	0.0011689	Paxs	391.17	Joback Method

dvisc	0.0007038	Paxs	431.92	Joback Method
dvisc	0.0004625	Paxs	472.66	Joback Method
dvisc	0.0003249	Paxs	513.40	Joback Method
dvisc	0.0002404	Paxs	554.15	Joback Method
dvisc	0.0001854	Paxs	594.89	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=U349027&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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