

Malonic acid, 2-chloropropyl octyl ester

Inchi:	InChI=1S/C14H25ClO4/c1-3-4-5-6-7-8-9-18-13(16)10-14(17)19-11-12(2)15/h12H,3-11H2
InchiKey:	DFJKJUMOXRTFSC-UHFFFAOYSA-N
Formula:	C14H25ClO4
SMILES:	CCCCCCCCOC(=O)CC(=O)OCC(C)Cl
Mol. weight [g/mol]:	292.80

Physical Properties

Property code	Value	Unit	Source
gf	-415.21	kJ/mol	Joback Method
hf	-842.91	kJ/mol	Joback Method
hfus	38.26	kJ/mol	Joback Method
hvap	69.07	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.451		Crippen Method
mvol	235.240	ml/mol	McGowan Method
pc	1601.28	kPa	Joback Method
rinpol	1908.00		NIST Webbook
rinpol	1908.00		NIST Webbook
tb	709.29	K	Joback Method
tc	892.20	K	Joback Method
tf	406.78	K	Joback Method
vc	0.910	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.17	J/molxK	709.29	Joback Method
cpg	668.23	J/molxK	739.77	Joback Method
cpg	682.49	J/molxK	770.26	Joback Method
cpg	695.99	J/molxK	800.74	Joback Method
cpg	708.71	J/molxK	831.23	Joback Method
cpg	720.66	J/molxK	861.71	Joback Method
cpg	731.86	J/molxK	892.20	Joback Method
dvisc	0.0014710	Paxs	406.78	Joback Method

dvisc	0.0007320	Paxs	457.20	Joback Method
dvisc	0.0004184	Paxs	507.62	Joback Method
dvisc	0.0002646	Paxs	558.03	Joback Method
dvisc	0.0001806	Paxs	608.45	Joback Method
dvisc	0.0001306	Paxs	658.87	Joback Method
dvisc	0.0000989	Paxs	709.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349030&Units=SI
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

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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