Malonic acid, di(2,2-dichloroethyl) ester

Inchi: InChI=1S/C7H8Cl4O4/c8-4(9)2-14-6(12)1-7(13)15-3-5(10)11/h4-5H,1-3H2
InchiKey: RYOQIENTSXLUNE-UHFFFAOYSA-N
Formula: C7H8Cl4O4
SMILES: O=C(CC(=O)OCC(Cl)Cl)OCC(Cl)Cl
Mol. weight [g/mol]: 297.95

Physical Properties

Property code	Value	Unit	Source
gf	-512.38	kJ/mol	Joback Method
hf	-750.93	kJ/mol	Joback Method
hfus	29.20	kJ/mol	Joback Method
hvap	66.25	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.070		Crippen Method
mcvol	173.330	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
rinpol	1765.00		NIST Webbook
tb	660.98	K	Joback Method
tc	871.39	K	Joback Method
tf	402.65	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.69	J/mol×K	660.98	Joback Method
cpg	379.29	J/mol×K	696.05	Joback Method
cpg	387.32	J/mol×K	731.12	Joback Method
cpg	394.79	J/mol×K	766.19	Joback Method
cpg	401.68	J/mol×K	801.26	Joback Method
cpg	407.99	J/mol×K	836.32	Joback Method
cpg	413.72	J/mol×K	871.39	Joback Method
dvisc	0.0017837	Pa×s	402.65	Joback Method
dvisc	0.0009869	Pa×s	445.71	Joback Method

dvisc	0.0006061	Pa×s	488.76	Joback Method
dvisc	0.0004028	Pa×s	531.82	Joback Method
dvisc	0.0002845	Pa×s	574.87	Joback Method
dvisc	0.0002110	Pa×s	617.93	Joback Method
dvisc	0.0001627	Pa×s	660.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349066&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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