Diethylmalonic acid, monochloride, 2,2-dichloroethyl ester

Inchi: InChI=1S/C9H13Cl3O3/c1-3-9(4-2,7(12)13)8(14)15-5-6(10)11/h6H,3-5H2,1-2H3

InchiKey: CECXJNPFGGUCOD-UHFFFAOYSA-N

Formula: C9H13Cl3O3

SMILES: CCC(CC)(C(=O)Cl)C(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 275.56

Physical Properties

Property code	Value	Unit	Source
gf	-373.33	kJ/mol	Joback Method
hf	-647.72	kJ/mol	Joback Method
hfus	25.11	kJ/mol	Joback Method
hvap	63.00	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.905		Crippen Method
mcvol	183.400	ml/mol	McGowan Method
pc	2363.37	kPa	Joback Method
rinpol	1481.00		NIST Webbook
rinpol	1481.00		NIST Webbook
tb	644.10	K	Joback Method
tc	854.01	K	Joback Method
tf	390.46	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.59	J/mol×K	644.10	Joback Method
cpg	473.15	J/mol×K	819.03	Joback Method
cpg	464.81	J/mol×K	784.04	Joback Method
cpg	455.82	J/mol×K	749.06	Joback Method
cpg	446.14	J/mol×K	714.07	Joback Method
cpg	435.74	J/mol×K	679.09	Joback Method
cpg	480.87	J/mol×K	854.01	Joback Method
dvisc	0.0001716	Pa×s	644.10	Joback Method

dvisc	0.0002270	Pa×s	601.83	Joback Method
dvisc	0.0003132	Pa×s	559.55	Joback Method
dvisc	0.0004555	Pa×s	517.28	Joback Method
dvisc	0.0007081	Pa×s	475.01	Joback Method
dvisc	0.0011999	Pa×s	432.73	Joback Method
dvisc	0.0022793	Pa×s	390.46	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=U370791&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