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

Inchi: InChI=1S/C11H16Cl4O4/c1-3-11(4-2,9(16)18-5-7(12)13)10(17)19-6-8(14)15/h7-8H,3-6H
InchiKey: AGLZFPQMUMSPAI-UHFFFAOYSA-N
Formula: C11H16Cl4O4
SMILES: CCC(CC)(C(=O)OCC(Cl)Cl)C(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 354.05

Physical Properties

Property code	Value	Unit	Source
gf	-475.86	kJ/mol	Joback Method
hf	-842.24	kJ/mol	Joback Method
hfus	32.15	kJ/mol	Joback Method
hvap	73.86	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.487		Crippen Method
mcvol	229.690	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	1874.00		NIST Webbook
rinpol	1874.00		NIST Webbook
tb	749.27	K	Joback Method
tc	958.62	K	Joback Method
tf	450.15	K	Joback Method
vc	0.873	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.81	J/mol×K	749.27	Joback Method
cpg	585.12	J/mol×K	784.16	Joback Method
cpg	595.59	J/mol×K	819.05	Joback Method
cpg	605.25	J/mol×K	853.95	Joback Method
cpg	614.13	J/mol×K	888.84	Joback Method
cpg	622.26	J/mol×K	923.73	Joback Method
cpg	629.65	J/mol×K	958.62	Joback Method
dvisc	0.0011569	Pa×s	450.15	Joback Method

dvisc	0.0005843	Pa×s	500.00	Joback Method
dvisc	0.0003340	Pa×s	549.86	Joback Method
dvisc	0.0002095	Pa×s	599.71	Joback Method
dvisc	0.0001412	Pa×s	649.56	Joback Method
dvisc	0.0001007	Pa×s	699.42	Joback Method
dvisc	0.0000751	Pa×s	749.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370790&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