

Diethylmalonic acid, monochloride, 2,2,2-trichloroethyl ester

Inchi:	InChI=1S/C9H12Cl4O3/c1-3-8(4-2,6(10)14)7(15)16-5-9(11,12)13/h3-5H2,1-2H3
InchiKey:	OSZPCPWIAWYGCF-UHFFFAOYSA-N
Formula:	C9H12Cl4O3
SMILES:	CCC(CC)(C(=O)Cl)C(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]:	310.00

Physical Properties

Property code	Value	Unit	Source
gf	-379.98	kJ/mol	Joback Method
hf	-666.93	kJ/mol	Joback Method
hfus	25.41	kJ/mol	Joback Method
hvap	66.48	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.472		Crippen Method
mvol	195.640	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
rinpol	1531.00		NIST Webbook
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tb	678.74	K	Joback Method
tc	899.46	K	Joback Method
tf	437.80	K	Joback Method
vc	0.744	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.11	J/molxK	678.74	Joback Method
cpg	460.37	J/molxK	715.53	Joback Method
cpg	469.79	J/molxK	752.31	Joback Method
cpg	478.45	J/molxK	789.10	Joback Method
cpg	486.39	J/molxK	825.89	Joback Method
cpg	493.69	J/molxK	862.68	Joback Method
cpg	500.39	J/molxK	899.46	Joback Method
dvisc	0.0014796	Paxs	437.80	Joback Method

dvisc	0.0008418	Paxs	477.96	Joback Method
dvisc	0.0005227	Paxs	518.11	Joback Method
dvisc	0.0003476	Paxs	558.27	Joback Method
dvisc	0.0002442	Paxs	598.43	Joback Method
dvisc	0.0001793	Paxs	638.58	Joback Method
dvisc	0.0001366	Paxs	678.74	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=U370472&Units=SI

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	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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