

Diethylmalonic acid, monochloride, 2-ethoxyethyl ester

Inchi:	InChI=1S/C11H19ClO4/c1-4-11(5-2,9(12)13)10(14)16-8-7-15-6-3/h4-8H2,1-3H3
InchiKey:	UXDKYJTWVBMUJP-UHFFFAOYSA-N
Formula:	C11H19ClO4
SMILES:	CCOCCOC(=O)C(CC)(CC)C(=O)Cl
Mol. weight [g/mol]:	250.72

Physical Properties

Property code	Value	Unit	Source
gf	-435.19	kJ/mol	Joback Method
hf	-784.46	kJ/mol	Joback Method
hfus	26.60	kJ/mol	Joback Method
hvap	61.48	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.138		Crippen Method
mcvol	192.970	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinsol	1409.00		NIST Webbook
tb	637.86	K	Joback Method
tc	829.59	K	Joback Method
tf	390.39	K	Joback Method
vc	0.738	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.77	J/molxK	637.86	Joback Method
cpg	558.10	J/molxK	797.63	Joback Method
cpg	547.25	J/molxK	765.68	Joback Method
cpg	535.70	J/molxK	733.72	Joback Method
cpg	523.45	J/molxK	701.77	Joback Method
cpg	510.48	J/molxK	669.81	Joback Method
cpg	568.26	J/molxK	829.59	Joback Method
dvisc	0.0001367	Paxs	637.86	Joback Method
dvisc	0.0001791	Paxs	596.61	Joback Method

dvisc	0.0002444	Paxs	555.37	Joback Method
dvisc	0.0003504	Paxs	514.12	Joback Method
dvisc	0.0005350	Paxs	472.88	Joback Method
dvisc	0.0008856	Paxs	431.63	Joback Method
dvisc	0.0016310	Paxs	390.39	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=U370619&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

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