

Octadecanoic acid, 9,10-dichloro-, methyl ester

Other names:	Methyl 9,10-dichlorooctadecanoate
Inchi:	InChI=1S/C19H36Cl2O2/c1-3-4-5-6-8-11-14-17(20)18(21)15-12-9-7-10-13-16-19(22)23-2
InchiKey:	KYPMPURXQCFWCJ-UHFFFAOYSA-N
Formula:	C19H36Cl2O2
SMILES:	CCCCCCCCC(Cl)C(Cl)CCCCCCCC(=O)OC
Mol. weight [g/mol]:	367.39
CAS:	33094-27-8

Physical Properties

Property code	Value	Unit	Source
gf	-153.56	kJ/mol	Joback Method
hf	-722.33	kJ/mol	Joback Method
hfus	49.10	kJ/mol	Joback Method
hvap	75.04	kJ/mol	Joback Method
log10ws	-7.17		Crippen Method
logp	6.856		Crippen Method
mcvol	310.490	ml/mol	McGowan Method
pc	1072.17	kPa	Joback Method
tb	784.39	K	Joback Method
tc	968.11	K	Joback Method
tf	405.89	K	Joback Method
vc	1.210	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.69	J/molxK	784.39	Joback Method
cpg	936.52	J/molxK	815.01	Joback Method
cpg	953.38	J/molxK	845.63	Joback Method
cpg	969.31	J/molxK	876.25	Joback Method
cpg	984.32	J/molxK	906.87	Joback Method
cpg	998.46	J/molxK	937.49	Joback Method
cpg	1011.74	J/molxK	968.11	Joback Method
dvisc	0.0016630	Paxs	405.89	Joback Method

dvisc	0.0006390	Paxs	468.97	Joback Method
dvisc	0.0003081	Paxs	532.06	Joback Method
dvisc	0.0001733	Paxs	595.14	Joback Method
dvisc	0.0001089	Paxs	658.22	Joback Method
dvisc	0.0000742	Paxs	721.31	Joback Method
dvisc	0.0000538	Paxs	784.39	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=C33094278&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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