

Diethylmalonic acid, monochloride, 2,6-dichlorophenyl ester

Inchi:	InChI=1S/C13H13Cl3O3/c1-3-13(4-2,11(16)17)12(18)19-10-8(14)6-5-7-9(10)15/h5-7H,3
InchiKey:	AMJJUTPUPNPMGX-UHFFFAOYSA-N
Formula:	C13H13Cl3O3
SMILES:	CCC(CC)(C(=O)Cl)C(=O)Oc1c(Cl)cccc1Cl
Mol. weight [g/mol]:	323.60

Physical Properties

Property code	Value	Unit	Source
gf	-244.06	kJ/mol	Joback Method
hf	-511.41	kJ/mol	Joback Method
hfus	32.25	kJ/mol	Joback Method
hvap	75.89	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.471		Crippen Method
mcvol	216.000	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpol	1995.00		NIST Webbook
tb	772.70	K	Joback Method
tc	1004.44	K	Joback Method
tf	502.00	K	Joback Method
vc	0.822	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.26	J/molxK	772.70	Joback Method
cpg	582.02	J/molxK	965.82	Joback Method
cpg	574.33	J/molxK	927.20	Joback Method
cpg	565.85	J/molxK	888.57	Joback Method
cpg	556.55	J/molxK	849.95	Joback Method
cpg	546.37	J/molxK	811.32	Joback Method
cpg	588.99	J/molxK	1004.44	Joback Method
dvisc	0.0001029	Paxs	772.70	Joback Method
dvisc	0.0001292	Paxs	727.58	Joback Method

dvisc	0.0001672	Paxs	682.47	Joback Method
dvisc	0.0002243	Paxs	637.35	Joback Method
dvisc	0.0003148	Paxs	592.23	Joback Method
dvisc	0.0004671	Paxs	547.12	Joback Method
dvisc	0.0007441	Paxs	502.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369946&Units=SI
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

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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