

Diethylmalonic acid, monochloride, 2,3,6-trichlorophenyl ester

Inchi:	InChI=1S/C13H12Cl4O3/c1-3-13(4-2,11(17)18)12(19)20-10-8(15)6-5-7(14)9(10)16/h5-6H
InchiKey:	LHLKBGNJSQZBPW-UHFFFAOYSA-N
Formula:	C13H12Cl4O3
SMILES:	CCC(CC)(C(=O)Cl)C(=O)Oc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]:	358.05

Physical Properties

Property code	Value	Unit	Source
gf	-265.62	kJ/mol	Joback Method
hf	-538.62	kJ/mol	Joback Method
hfus	36.06	kJ/mol	Joback Method
hvap	80.94	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	5.124		Crippen Method
mcvol	228.240	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinsol	2188.00		NIST Webbook
tb	815.11	K	Joback Method
tc	1050.07	K	Joback Method
tf	544.44	K	Joback Method
vc	0.871	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	554.02	J/molxK	815.11	Joback Method
cpg	563.93	J/molxK	854.27	Joback Method
cpg	572.96	J/molxK	893.43	Joback Method
cpg	581.16	J/molxK	932.59	Joback Method
cpg	588.57	J/molxK	971.75	Joback Method
cpg	595.24	J/molxK	1010.91	Joback Method
cpg	601.21	J/molxK	1050.07	Joback Method
dvisc	0.0005412	Paxs	544.44	Joback Method
dvisc	0.0003573	Paxs	589.55	Joback Method

dvisc	0.0002502	Paxs	634.66	Joback Method
dvisc	0.0001837	Paxs	679.77	Joback Method
dvisc	0.0001402	Paxs	724.89	Joback Method
dvisc	0.0001104	Paxs	770.00	Joback Method
dvisc	0.0000893	Paxs	815.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370291&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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