

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

Inchi:	InChI=1S/C16H19Cl3O4/c1-4-9-22-14(20)16(5-2,6-3)15(21)23-13-11(18)8-7-10(17)12(13)
InchiKey:	AEHDVLZVULHBSJ-UHFFFAOYSA-N
Formula:	C16H19Cl3O4
SMILES:	CCCOC(=O)C(CC)(CC)C(=O)Oc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]:	381.68

Physical Properties

Property code	Value	Unit	Source
gf	-333.43	kJ/mol	Joback Method
hf	-717.02	kJ/mol	Joback Method
hfus	40.82	kJ/mol	Joback Method
hvap	85.64	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.312		Crippen Method
mcvol	264.140	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
rinpol	2326.00		NIST Webbook
tb	868.74	K	Joback Method
tc	1090.97	K	Joback Method
tf	570.56	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.62	J/molxK	868.74	Joback Method
cpg	733.30	J/molxK	905.78	Joback Method
cpg	743.96	J/molxK	942.82	Joback Method
cpg	753.61	J/molxK	979.86	Joback Method
cpg	762.30	J/molxK	1016.89	Joback Method
cpg	770.05	J/molxK	1053.93	Joback Method
cpg	776.89	J/molxK	1090.97	Joback Method
dvisc	0.0003400	Paxs	570.56	Joback Method
dvisc	0.0002173	Paxs	620.26	Joback Method

dvisc	0.0001484	Paxs	669.95	Joback Method
dvisc	0.0001069	Paxs	719.65	Joback Method
dvisc	0.0000803	Paxs	769.35	Joback Method
dvisc	0.0000624	Paxs	819.04	Joback Method
dvisc	0.0000500	Paxs	868.74	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=U370282&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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