

Diethylmalonic acid, di(2,3-dichlorophenyl) ester

Inchi:	InChI=1S/C19H16Cl4O4/c1-3-19(4-2,17(24)26-13-9-5-7-11(20)15(13)22)18(25)27-14-10
InchiKey:	VNWNVBODHMJMLB-UHFFFAOYSA-N
Formula:	C19H16Cl4O4
SMILES:	CCC(CC)(C(=O)Oc1cccc(Cl)c1Cl)C(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	450.14

Physical Properties

Property code	Value	Unit	Source
gf	-217.32	kJ/mol	Joback Method
hf	-569.62	kJ/mol	Joback Method
hfus	46.44	kJ/mol	Joback Method
hvap	99.64	kJ/mol	Joback Method
log10ws	-7.50		Crippen Method
logp	6.618		Crippen Method
mcvol	294.890	ml/mol	McGowan Method
pc	1629.85	kPa	Joback Method
rinpol	2982.00		NIST Webbook
rinpol	2982.00		NIST Webbook
tb	1006.47	K	Joback Method
tc	1255.53	K	Joback Method
tf	673.23	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	801.39	J/molxK	1006.47	Joback Method
cpg	833.56	J/molxK	1214.02	Joback Method
cpg	829.20	J/molxK	1172.51	Joback Method
cpg	823.86	J/molxK	1131.00	Joback Method
cpg	817.49	J/molxK	1089.49	Joback Method
cpg	810.02	J/molxK	1047.98	Joback Method
cpg	837.01	J/molxK	1255.53	Joback Method
dvisc	0.0000278	Paxs	1006.47	Joback Method

dvisc	0.0000344	Paxs	950.93	Joback Method
dvisc	0.0000435	Paxs	895.39	Joback Method
dvisc	0.0000569	Paxs	839.85	Joback Method
dvisc	0.0000772	Paxs	784.31	Joback Method
dvisc	0.0001098	Paxs	728.77	Joback Method
dvisc	0.0001654	Paxs	673.23	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370045&Units=SI

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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