

Diethylmalonic acid, di(2,3,5-trichlorophenyl) ester

Inchi:	InChI=1S/C19H14Cl6O4/c1-3-19(4-2,17(26)28-13-7-9(20)5-11(22)15(13)24)18(27)29-14
InchiKey:	HDUGZLQDXXXINH-UHFFFAOYSA-N
Formula:	C19H14Cl6O4
SMILES:	CCC(CC)(C(=O)Oc1cc(Cl)cc(Cl)c1Cl)C(=O)Oc1cc(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	519.03

Physical Properties

Property code	Value	Unit	Source
gf	-260.44	kJ/mol	Joback Method
hf	-624.04	kJ/mol	Joback Method
hfus	54.06	kJ/mol	Joback Method
hvap	109.74	kJ/mol	Joback Method
log10ws	-8.87		Crippen Method
logp	7.924		Crippen Method
mcvol	319.370	ml/mol	McGowan Method
pc	1501.15	kPa	Joback Method
rinpol	3165.00		NIST Webbook
rinpol	3165.00		NIST Webbook
tb	1091.29	K	Joback Method
tc	1349.43	K	Joback Method
tf	758.11	K	Joback Method
vc	1.214	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.91	J/molxK	1091.29	Joback Method
cpg	832.76	J/molxK	1134.31	Joback Method
cpg	837.44	J/molxK	1177.34	Joback Method
cpg	841.02	J/molxK	1220.36	Joback Method
cpg	843.54	J/molxK	1263.38	Joback Method
cpg	845.06	J/molxK	1306.40	Joback Method
cpg	845.64	J/molxK	1349.43	Joback Method
dvisc	0.0000961	Paxs	758.11	Joback Method

dvisc	0.0000678	Paxs	813.64	Joback Method
dvisc	0.0000501	Paxs	869.17	Joback Method
dvisc	0.0000384	Paxs	924.70	Joback Method
dvisc	0.0000303	Paxs	980.23	Joback Method
dvisc	0.0000245	Paxs	1035.76	Joback Method
dvisc	0.0000203	Paxs	1091.29	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=U370557&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
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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