

m,p'-DDT

Inchi:	InChI=1S/C14H9Cl5/c15-11-6-4-9(5-7-11)13(14(17,18)19)10-2-1-3-12(16)8-10/h1-8,13H
InchiKey:	LMNGXUAFBMMCLT-UHFFFAOYSA-N
Formula:	C14H9Cl5
SMILES:	Clc1ccc(C(c2cccc(Cl)c2)C(Cl)(Cl)Cl)cc1
Mol. weight [g/mol]:	354.49

Physical Properties

Property code	Value	Unit	Source
gf	213.31	kJ/mol	Joback Method
hf	25.10	kJ/mol	Joback Method
hfus	29.37	kJ/mol	Joback Method
hvap	72.88	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	6.495		Crippen Method
mcvol	221.800	ml/mol	McGowan Method
pc	2293.71	kPa	Joback Method
rinqol	2332.00		NIST Webbook
tb	766.52	K	Joback Method
tc	1041.34	K	Joback Method
tf	462.44	K	Joback Method
vc	0.832	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.29	J/molxK	766.52	Joback Method
cpg	541.13	J/molxK	995.53	Joback Method
cpg	533.67	J/molxK	949.73	Joback Method
cpg	525.51	J/molxK	903.93	Joback Method
cpg	516.50	J/molxK	858.13	Joback Method
cpg	506.48	J/molxK	812.32	Joback Method
cpg	548.06	J/molxK	1041.34	Joback Method
dvisc	0.0000899	Paxs	766.52	Joback Method
dvisc	0.0001157	Paxs	715.84	Joback Method

dvisc	0.0001547	Paxs	665.16	Joback Method
dvisc	0.0002169	Paxs	614.48	Joback Method
dvisc	0.0003233	Paxs	563.80	Joback Method
dvisc	0.0005214	Paxs	513.12	Joback Method
dvisc	0.0009338	Paxs	462.44	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=R547510&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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