

Dichlorophen, O-(isobutyryl)-

Inchi:	InChI=1S/C17H16Cl2O3/c1-10(2)17(21)22-16-6-4-14(19)9-12(16)7-11-8-13(18)3-5-15(1
InchiKey:	XTXMWYHFJPFIXIN-UHFFFAOYSA-N
Formula:	C17H16Cl2O3
SMILES:	CC(C)C(=O)Oc1ccc(Cl)cc1Cc1cc(Cl)ccc1O
Mol. weight [g/mol]:	339.21

Physical Properties

Property code	Value	Unit	Source
gf	-126.65	kJ/mol	Joback Method
hf	-414.43	kJ/mol	Joback Method
hfus	40.14	kJ/mol	Joback Method
hvap	90.53	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	4.851		Crippen Method
mvol	240.660	ml/mol	McGowan Method
pc	2258.96	kPa	Joback Method
rinpol	2600.00		NIST Webbook
tb	887.99	K	Joback Method
tc	1134.27	K	Joback Method
tf	600.47	K	Joback Method
vc	0.854	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.37	J/molxK	887.99	Joback Method
cpg	677.68	J/molxK	929.04	Joback Method
cpg	689.22	J/molxK	970.08	Joback Method
cpg	700.12	J/molxK	1011.13	Joback Method
cpg	710.46	J/molxK	1052.17	Joback Method
cpg	720.37	J/molxK	1093.22	Joback Method
cpg	729.95	J/molxK	1134.27	Joback Method
dvisc	0.0000569	Paxs	600.47	Joback Method
dvisc	0.0000304	Paxs	648.39	Joback Method

dvisc	0.0000177	Paxs	696.31	Joback Method
dvisc	0.0000111	Paxs	744.23	Joback Method
dvisc	0.0000073	Paxs	792.15	Joback Method
dvisc	0.0000051	Paxs	840.07	Joback Method
dvisc	0.0000037	Paxs	887.99	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=U354643&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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