

Dichlorphen, O-isovaleryl-

Inchi:	InChI=1S/C18H18Cl2O3/c1-11(2)7-18(22)23-17-6-4-15(20)10-13(17)8-12-9-14(19)3-5-16
InchiKey:	HQWCCOALJIAXON-UHFFFAOYSA-N
Formula:	C18H18Cl2O3
SMILES:	CC(C)CC(=O)Oc1ccc(Cl)cc1Cc1cc(Cl)ccc1O
Mol. weight [g/mol]:	353.24

Physical Properties

Property code	Value	Unit	Source
gf	-118.23	kJ/mol	Joback Method
hf	-435.07	kJ/mol	Joback Method
hfus	42.73	kJ/mol	Joback Method
hvap	92.75	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	5.241		Crippen Method
mvol	254.750	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	2666.00		NIST Webbook
rinpol	2666.00		NIST Webbook
tb	910.87	K	Joback Method
tc	1153.76	K	Joback Method
tf	611.74	K	Joback Method
vc	0.909	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.81	J/molxK	910.87	Joback Method
cpg	778.93	J/molxK	1113.28	Joback Method
cpg	768.58	J/molxK	1072.79	Joback Method
cpg	757.80	J/molxK	1032.31	Joback Method
cpg	746.48	J/molxK	991.83	Joback Method
cpg	734.52	J/molxK	951.35	Joback Method
cpg	788.96	J/molxK	1153.76	Joback Method
dvisc	0.0000030	Paxs	910.87	Joback Method

dvisc	0.0000042	Paxs	861.01	Joback Method
dvisc	0.0000060	Paxs	811.16	Joback Method
dvisc	0.0000092	Paxs	761.30	Joback Method
dvisc	0.0000148	Paxs	711.45	Joback Method
dvisc	0.0000256	Paxs	661.60	Joback Method
dvisc	0.0000485	Paxs	611.74	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=U360661&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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