

Dichlorophene, O,O'-di(3-methylbut-2-enoyl)-

Other names:	Dichlorophen, O,O'-di(3-methylbut-2-enoyl)-
Inchi:	InChI=1S/C23H22Cl2O4/c1-14(2)9-22(26)28-20-7-5-18(24)12-16(20)11-17-13-19(25)6-8
InchiKey:	LVDOXQUBTQZYRA-UHFFFAOYSA-N
Formula:	C23H22Cl2O4
SMILES:	CC(C)=CC(=O)Oc1ccc(Cl)cc1Cc1cc(Cl)ccc1OC(=O)C=C(C)C
Mol. weight [g/mol]:	433.32

Physical Properties

Property code	Value	Unit	Source
gf	-19.28	kJ/mol	Joback Method
hf	-397.09	kJ/mol	Joback Method
hfus	53.60	kJ/mol	Joback Method
hvap	101.15	kJ/mol	Joback Method
log10ws	-7.79		Crippen Method
logp	6.327		Crippen Method
mcvol	318.170	ml/mol	McGowan Method
pc	1379.91	kPa	Joback Method
rinpol	3021.00		NIST Webbook
rinpol	3021.00		NIST Webbook
tb	1034.44	K	Joback Method
tc	1279.82	K	Joback Method
tf	617.97	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.22	J/molxK	1034.44	Joback Method
cpg	948.80	J/molxK	1075.34	Joback Method
cpg	959.30	J/molxK	1116.23	Joback Method
cpg	968.81	J/molxK	1157.13	Joback Method
cpg	977.41	J/molxK	1198.03	Joback Method
cpg	985.18	J/molxK	1238.93	Joback Method
cpg	992.21	J/molxK	1279.82	Joback Method

Sources

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=U355135&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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