

Spirodiclofen

Inchi:	InChI=1S/C21H24Cl2O4/c1-4-20(2,3)19(25)26-17-16(14-9-8-13(22)12-15(14)23)18(24)2
InchiKey:	DTDSAWVUFPGDMX-UHFFFAOYSA-N
Formula:	C21H24Cl2O4
SMILES:	CCC(C)(C)C(=O)OC1=C(c2ccc(Cl)cc2Cl)C(=O)OC12CCCCC2
Mol. weight [g/mol]:	411.32

Physical Properties

Property code	Value	Unit	Source
gf	-158.54	kJ/mol	Joback Method
hf	-626.53	kJ/mol	Joback Method
hfus	35.61	kJ/mol	Joback Method
hvap	92.61	kJ/mol	Joback Method
log10ws	-6.99		Crippen Method
logp	5.944		Crippen Method
mvol	296.330	ml/mol	McGowan Method
pc	1636.45	kPa	Joback Method
rinpol	2690.00		NIST Webbook
rinpol	2690.00		NIST Webbook
tb	1003.80	K	Joback Method
tc	1263.89	K	Joback Method
tf	682.84	K	Joback Method
vc	1.109	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	953.89	J/mol×K	1003.80	Joback Method
cpg	973.06	J/mol×K	1047.15	Joback Method
cpg	992.10	J/mol×K	1090.50	Joback Method
cpg	1011.25	J/mol×K	1133.84	Joback Method
cpg	1030.74	J/mol×K	1177.19	Joback Method
cpg	1050.81	J/mol×K	1220.54	Joback Method
cpg	1071.68	J/mol×K	1263.89	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R566764&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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