

Acifluorfen, nonyl ester

Inchi:	InChI=1S/C23H25ClF3NO5/c1-2-3-4-5-6-7-8-13-32-22(29)18-15-17(10-11-20(18)28(30)31)
InchiKey:	OJOAJBJSUPZILK-UHFFFAOYSA-N
Formula:	C23H25ClF3NO5
SMILES:	CCCCCCCCCOC(=O)c1cc(Oc2ccc(C(F)(F)F)cc2Cl)ccc1[N+](=O)[O-]
Mol. weight [g/mol]:	487.90

Physical Properties

Property code	Value	Unit	Source
gf	-567.81	kJ/mol	Joback Method
hf	-1091.47	kJ/mol	Joback Method
hfus	63.21	kJ/mol	Joback Method
hvap	102.79	kJ/mol	Joback Method
log10ws	-9.14		Crippen Method
logp	7.967		Crippen Method
mvol	335.690	ml/mol	McGowan Method
pc	1160.08	kPa	Joback Method
rinpol	3315.00		NIST Webbook
rinpol	3315.00		NIST Webbook
tb	1081.48	K	Joback Method
tc	1324.47	K	Joback Method
tf	724.00	K	Joback Method
vc	1.323	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1084.88	J/mol×K	1081.48	Joback Method
cpg	1095.23	J/mol×K	1121.98	Joback Method
cpg	1104.31	J/mol×K	1162.48	Joback Method
cpg	1112.21	J/mol×K	1202.98	Joback Method
cpg	1119.02	J/mol×K	1243.47	Joback Method
cpg	1124.83	J/mol×K	1283.97	Joback Method
cpg	1129.71	J/mol×K	1324.47	Joback Method

Sources

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=U415148&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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