Acifluorfen, octyl ester

Inchi: InChI=1S/C22H23ClF3NO5/c1-2-3-4-5-6-7-12-31-21(28)17-14-16(9-10-19(17)27(29)30)3
InchiKey: XYFLXYKWYLMEJB-UHFFFAOYSA-N
Formula: C22H23ClF3NO5
SMILES: CCCCCCCCOC(=O)c1cc(Oc2ccc(C(F)(F)F)cc2Cl)ccc1[N+](=O)[O-]
Mol. weight [g/mol]: 473.87

Physical Properties

Property code	Value	Unit	Source
gf	-576.23	kJ/mol	Joback Method
hf	-1070.83	kJ/mol	Joback Method
hfus	60.62	kJ/mol	Joback Method
hvap	100.56	kJ/mol	Joback Method
log10ws	-8.72		Crippen Method
logp	7.577		Crippen Method
mcvol	321.600	ml/mol	McGowan Method
pc	1239.83	kPa	Joback Method
rinpol	3213.00		NIST Webbook
tb	1058.60	K	Joback Method
tc	1298.00	K	Joback Method
tf	712.73	K	Joback Method
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1025.64	J/mol×K	1058.60	Joback Method
cpg	1035.81	J/mol×K	1098.50	Joback Method
cpg	1044.76	J/mol×K	1138.40	Joback Method
cpg	1052.56	J/mol×K	1178.30	Joback Method
cpg	1059.29	J/mol×K	1218.20	Joback Method
cpg	1065.03	J/mol×K	1258.10	Joback Method
cpg	1069.85	J/mol×K	1298.00	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=U415147&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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