Acifluorfen, undecyl ester

Inchi: InChI=1S/C25H29ClF3NO5/c1-2-3-4-5-6-7-8-9-10-15-34-24(31)20-17-19(12-13-22(20)30
InchiKey: QCBMFQQJCBVDDB-UHFFFAOYSA-N
Formula: C25H29ClF3NO5
SMILES: CCCCCCCCCCCOC(=O)c1cc(Oc2ccc(C(F)(F)F)cc2Cl)ccc1[N+](=O)[O-]
Mol. weight [g/mol]: 515.95

Physical Properties

Property code	Value	Unit	Source
gf	-550.97	kJ/mol	Joback Method
hf	-1132.75	kJ/mol	Joback Method
hfus	68.39	kJ/mol	Joback Method
hvap	107.24	kJ/mol	Joback Method
log10ws	-9.97		Crippen Method
logp	8.747		Crippen Method
mcvol	363.870	ml/mol	McGowan Method
pc	1022.04	kPa	Joback Method
rinpol	3517.00		NIST Webbook
tb	1127.24	K	Joback Method
tc	1380.83	K	Joback Method
tf	746.54	K	Joback Method
vc	1.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1204.67	J/mol×K	1127.24	Joback Method
cpg	1215.41	J/mol×K	1169.51	Joback Method
cpg	1224.79	J/mol×K	1211.77	Joback Method
cpg	1232.92	J/mol×K	1254.04	Joback Method
cpg	1239.90	J/mol×K	1296.30	Joback Method
cpg	1245.86	J/mol×K	1338.57	Joback Method
cpg	1250.88	J/mol×K	1380.83	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=U415150&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