Acifluorfen, pentyl ester

Inchi: InChI=1S/C19H17ClF3NO5/c1-2-3-4-9-28-18(25)14-11-13(6-7-16(14)24(26)27)29-17-8-5
InchiKey: ZLDJJDHUCWYLJN-UHFFFAOYSA-N
Formula: C19H17ClF3NO5
SMILES: CCCCCOC(=O)c1cc(Oc2ccc(C(F)(F)F)cc2Cl)ccc1[N+](=O)[O-]
Mol. weight [g/mol]: 431.79

Physical Properties

Property code	Value	Unit	Source
gf	-601.49	kJ/mol	Joback Method
hf	-1008.91	kJ/mol	Joback Method
hfus	52.85	kJ/mol	Joback Method
hvap	93.88	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	6.406		Crippen Method
mcvol	279.330	ml/mol	McGowan Method
pc	1535.46	kPa	Joback Method
rinpol	2904.00		NIST Webbook
rinpol	2904.00		NIST Webbook
tb	989.96	K	Joback Method
tc	1224.68	K	Joback Method
tf	678.92	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.94	J/mol×K	989.96	Joback Method
cpg	860.64	J/mol×K	1029.08	Joback Method
cpg	869.20	J/mol×K	1068.20	Joback Method
cpg	876.67	J/mol×K	1107.32	Joback Method
cpg	883.12	J/mol×K	1146.44	Joback Method
cpg	888.60	J/mol×K	1185.56	Joback Method
cpg	893.18	J/mol×K	1224.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415144&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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