Acifluorfen, hexyl ester

Inchi: InChI=1S/C20H19ClF3NO5/c1-2-3-4-5-10-29-19(26)15-12-14(7-8-17(15)25(27)28)30-18-
InchiKey: IMLYIJVDPOQDHQ-UHFFFAOYSA-N
Formula: C20H19ClF3NO5
SMILES: CCCCCCOC(=O)c1cc(Oc2ccc(C(F)(F)F)cc2Cl)ccc1[N+](=O)[O-]
Mol. weight [g/mol]: 445.82

Physical Properties

Property code	Value	Unit	Source
gf	-593.07	kJ/mol	Joback Method
hf	-1029.55	kJ/mol	Joback Method
hfus	55.44	kJ/mol	Joback Method
hvap	96.11	kJ/mol	Joback Method
log10ws	-7.88		Crippen Method
logp	6.796		Crippen Method
mcvol	293.420	ml/mol	McGowan Method
pc	1426.15	kPa	Joback Method
rinpol	3007.00		NIST Webbook
tb	1012.84	K	Joback Method
tc	1248.17	K	Joback Method
tf	690.19	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.63	J/mol×K	1012.84	Joback Method
cpg	918.48	J/mol×K	1052.06	Joback Method
cpg	927.18	J/mol×K	1091.28	Joback Method
cpg	934.77	J/mol×K	1130.50	Joback Method
cpg	941.32	J/mol×K	1169.72	Joback Method
cpg	946.90	J/mol×K	1208.94	Joback Method
cpg	951.58	J/mol×K	1248.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415145&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