Acifluorfen, propyl ester

Inchi: InChI=1S/C17H13ClF3NO5/c1-2-7-26-16(23)12-9-11(4-5-14(12)22(24)25)27-15-6-3-10(8
InchiKey: ZZCKHVXKCLNEAW-UHFFFAOYSA-N
Formula: C17H13ClF3NO5
SMILES: CCCOC(=O)c1cc(Oc2ccc(C(F)(F)F)cc2Cl)ccc1[N+](=O)[O-]
Mol. weight [g/mol]: 403.74

Physical Properties

Property code	Value	Unit	Source
gf	-618.33	kJ/mol	Joback Method
hf	-967.63	kJ/mol	Joback Method
hfus	47.67	kJ/mol	Joback Method
hvap	89.43	kJ/mol	Joback Method
log10ws	-6.63		Crippen Method
logp	5.626		Crippen Method
mcvol	251.150	ml/mol	McGowan Method
pc	1795.46	kPa	Joback Method
rinpol	2611.00		NIST Webbook
rinpol	2611.00		NIST Webbook
tb	944.20	K	Joback Method
tc	1180.31	K	Joback Method
tf	656.38	K	Joback Method
vc	0.988	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.45	J/mol×K	944.20	Joback Method
cpg	746.79	J/mol×K	983.55	Joback Method
cpg	755.02	J/mol×K	1022.90	Joback Method
cpg	762.20	J/mol×K	1062.26	Joback Method
cpg	768.37	J/mol×K	1101.61	Joback Method
cpg	773.59	J/mol×K	1140.96	Joback Method
cpg	777.92	J/mol×K	1180.31	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=U415141&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