Acifluorfen, isobutyl ester

Inchi: InChI=1S/C18H15ClF3NO5/c1-10(2)9-27-17(24)13-8-12(4-5-15(13)23(25)26)28-16-6-3-1
InchiKey: IHGLAZUWEBNZJM-UHFFFAOYSA-N
Formula: C18H15ClF3NO5
SMILES: CC(C)COC(=O)c1cc(Oc2ccc(C(F)(F)F)cc2Cl)ccc1[N+](=O)[O-]
Mol. weight [g/mol]: 417.76

Physical Properties

Property code	Value	Unit	Source
gf	-612.35	kJ/mol	Joback Method
hf	-993.55	kJ/mol	Joback Method
hfus	46.74	kJ/mol	Joback Method
hvap	91.27	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	5.872		Crippen Method
mcvol	265.240	ml/mol	McGowan Method
pc	1668.70	kPa	Joback Method
rinpol	2710.00		NIST Webbook
rinpol	2710.00		NIST Webbook
tb	966.64	K	Joback Method
tc	1204.03	K	Joback Method
tf	652.65	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.35	J/mol×K	966.64	Joback Method
cpg	803.91	J/mol×K	1006.21	Joback Method
cpg	812.31	J/mol×K	1045.77	Joback Method
cpg	819.60	J/mol×K	1085.34	Joback Method
cpg	825.85	J/mol×K	1124.90	Joback Method
cpg	831.10	J/mol×K	1164.47	Joback Method
cpg	835.43	J/mol×K	1204.03	Joback Method

Sources

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=U415142&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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