Acifluorfen, butyl ester

Inchi: InChI=1S/C18H15ClF3NO5/c1-2-3-8-27-17(24)13-10-12(5-6-15(13)23(25)26)28-16-7-4-1
InchiKey: PIWYWRFEDQYIEK-UHFFFAOYSA-N
Formula: C18H15ClF3NO5
SMILES: CCCCOC(=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	-609.91	kJ/mol	Joback Method
hf	-988.27	kJ/mol	Joback Method
hfus	50.26	kJ/mol	Joback Method
hvap	91.66	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	6.016		Crippen Method
mcvol	265.240	ml/mol	McGowan Method
pc	1657.84	kPa	Joback Method
rinpol	2806.00		NIST Webbook
rinpol	2806.00		NIST Webbook
tb	967.08	K	Joback Method
tc	1202.08	K	Joback Method
tf	667.65	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.87	J/mol×K	967.08	Joback Method
cpg	803.40	J/mol×K	1006.25	Joback Method
cpg	811.80	J/mol×K	1045.41	Joback Method
cpg	819.14	J/mol×K	1084.58	Joback Method
cpg	825.46	J/mol×K	1123.74	Joback Method
cpg	830.83	J/mol×K	1162.91	Joback Method
cpg	835.29	J/mol×K	1202.08	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=U415143&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