Acifluorfen, dodecyl ester

Inchi: InChI=1S/C26H31ClF3NO5/c1-2-3-4-5-6-7-8-9-10-11-16-35-25(32)21-18-20(13-14-23(21
InchiKey: VRASPOILRCZLKZ-UHFFFAOYSA-N
Formula: C26H31ClF3NO5
SMILES: CCCCCCCCCCCCOC(=O)c1cc(Oc2ccc(C(F)(F)F)cc2Cl)ccc1[N+](=O)[O-]
Mol. weight [g/mol]: 529.98

Physical Properties

Property code	Value	Unit	Source
gf	-542.55	kJ/mol	Joback Method
hf	-1153.39	kJ/mol	Joback Method
hfus	70.98	kJ/mol	Joback Method
hvap	109.46	kJ/mol	Joback Method
log10ws	-10.39		Crippen Method
logp	9.137		Crippen Method
mcvol	377.960	ml/mol	McGowan Method
pc	962.08	kPa	Joback Method
rinpol	3622.00		NIST Webbook
rinpol	3622.00		NIST Webbook
tb	1150.12	K	Joback Method
tc	1410.87	K	Joback Method
tf	757.81	K	Joback Method
vc	1.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1265.16	J/mol×K	1150.12	Joback Method
cpg	1276.12	J/mol×K	1193.58	Joback Method
cpg	1285.68	J/mol×K	1237.04	Joback Method
cpg	1293.94	J/mol×K	1280.50	Joback Method
cpg	1301.04	J/mol×K	1323.96	Joback Method
cpg	1307.08	J/mol×K	1367.42	Joback Method
cpg	1312.21	J/mol×K	1410.87	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415151&Units=SI

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