Acifluorfen, decyl ester

Inchi: InChI=1S/C24H27ClF3NO5/c1-2-3-4-5-6-7-8-9-14-33-23(30)19-16-18(11-12-21(19)29(31
InchiKey: AQYQWMUOAATUAK-UHFFFAOYSA-N
Formula: C24H27ClF3NO5
SMILES: CCCCCCCCCCOC(=O)c1cc(Oc2ccc(C(F)(F)F)cc2Cl)ccc1[N+](=O)[O-]
Mol. weight [g/mol]: 501.92

Physical Properties

Property code	Value	Unit	Source
gf	-559.39	kJ/mol	Joback Method
hf	-1112.11	kJ/mol	Joback Method
hfus	65.80	kJ/mol	Joback Method
hvap	105.01	kJ/mol	Joback Method
log10ws	-9.56		Crippen Method
logp	8.357		Crippen Method
mcvol	349.780	ml/mol	McGowan Method
pc	1087.78	kPa	Joback Method
rinpol	3417.00		NIST Webbook
tb	1104.36	K	Joback Method
tc	1352.06	K	Joback Method
tf	735.27	K	Joback Method
vc	1.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1144.57	J/mol×K	1104.36	Joback Method
cpg	1155.10	J/mol×K	1145.64	Joback Method
cpg	1164.32	J/mol×K	1186.93	Joback Method
cpg	1172.33	J/mol×K	1228.21	Joback Method
cpg	1179.23	J/mol×K	1269.49	Joback Method
cpg	1185.10	J/mol×K	1310.77	Joback Method
cpg	1190.05	J/mol×K	1352.06	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=U415149&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