

Acifluorfen, tridecyl ester

Inchi:	InChI=1S/C27H33CIF3NO5/c1-2-3-4-5-6-7-8-9-10-11-12-17-36-26(33)22-19-21(14-15-24
InchiKey:	LCCFAYQAVJTKPS-UHFFFAOYSA-N
Formula:	C27H33CIF3NO5
SMILES:	CCCCCCCCCCCCOC(=O)c1cc(Oc2ccc(C(F)(F)F)cc2Cl)ccc1[N+](=O)[O-]
Mol. weight [g/mol]:	544.00

Physical Properties

Property code	Value	Unit	Source
gf	-534.13	kJ/mol	Joback Method
hf	-1174.03	kJ/mol	Joback Method
hfus	73.57	kJ/mol	Joback Method
hvap	111.69	kJ/mol	Joback Method
log10ws	-10.81		Crippen Method
logp	9.527		Crippen Method
mvol	392.050	ml/mol	McGowan Method
pc	907.24	kPa	Joback Method
rinpol	2609.00		NIST Webbook
rinpol	2609.00		NIST Webbook
tb	1173.00	K	Joback Method
tc	1442.27	K	Joback Method
tf	769.08	K	Joback Method
vc	1.548	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1326.00	J/molxK	1173.00	Joback Method
cpg	1337.23	J/molxK	1217.88	Joback Method
cpg	1346.99	J/molxK	1262.76	Joback Method
cpg	1355.41	J/molxK	1307.63	Joback Method
cpg	1362.63	J/molxK	1352.51	Joback Method
cpg	1368.80	J/molxK	1397.39	Joback Method
cpg	1374.05	J/molxK	1442.27	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U415152&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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