

Acifluorfen

Other names:	Benzoic acid, 5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nitro-5-[2-Chloro-4-(trifluoromethyl)phenoxy]-2-nitrobenzoic acid Tackle 62476-59-9 (sodium salt)
Inchi:	InChI=1S/C14H7ClF3NO5/c15-10-5-7(14(16,17)18)1-4-12(10)24-8-2-3-11(19(22)23)9(6-
InchiKey:	NUFNQYOELLVIPL-UHFFFAOYSA-N
Formula:	C14H7ClF3NO5
SMILES:	O=C(O)c1cc(Oc2ccc(C(F)(F)F)cc2Cl)ccc1[N+](=O)[O-]
Mol. weight [g/mol]:	361.66
CAS:	50594-66-6

Physical Properties

Property code	Value	Unit	Source
gf	-675.41	kJ/mol	Joback Method
hf	-925.72	kJ/mol	Joback Method
hfus	42.80	kJ/mol	Joback Method
hvap	97.02	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.757		Crippen Method
mvol	208.880	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
rinpol	2903.00		NIST Webbook
rinpol	2903.00		NIST Webbook
tb	945.32	K	Joback Method
tc	1179.69	K	Joback Method
tf	437.48 ± 0.20	K	NIST Webbook
vc	0.821	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	613.09	J/mol×K	1140.63	Joback Method
cpg	586.60	J/mol×K	945.32	Joback Method
cpg	593.30	J/mol×K	984.38	Joback Method

cpg	599.24	J/mol×K	1023.44	Joback Method
cpg	604.47	J/mol×K	1062.50	Joback Method
cpg	609.07	J/mol×K	1101.56	Joback Method
cpg	616.59	J/mol×K	1179.69	Joback Method
hfust	37.67	kJ/mol	436.60	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50594666&Units=SI
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

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
hfust:	Enthalpy of fusion at a given temperature
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

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