Benzoic acid, 5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nitro-, ethyl ester

Other names: Ethyl 5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nitro-benzoate
Acifluorfen, ethyl ester

Inchi: InChI=1S/C16H11ClF3NO5/c1-2-25-15(22)11-8-10(4-5-13(11)21(23)24)26-14-6-3-9(7-12

InchiKey: ZXYLZOBDCIFSPF-UHFFFAOYSA-N

Formula: C16H11ClF3NO5

SMILES: CCOC(=O)c1cc(Oc2ccc(C(F)(F)F)cc2Cl)ccc1[N+](=O)[O-]

Mol. weight [g/mol]: 389.71

CAS: 77207-01-3

Physical Properties

Property code	Value	Unit	Source
gf	-626.75	kJ/mol	Joback Method
hf	-946.99	kJ/mol	Joback Method
hfus	45.08	kJ/mol	Joback Method
hvap	87.20	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	5.236		Crippen Method
mcvol	237.060	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	2304.00		NIST Webbook
rinpol	2304.00		NIST Webbook
tb	921.32	K	Joback Method
tc	1159.34	K	Joback Method
tf	645.11	K	Joback Method
vc	0.931	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.75	J/mol×K	921.32	Joback Method
cpg	690.87	J/mol×K	960.99	Joback Method
cpg	698.90	J/mol×K	1000.66	Joback Method
cpg	705.88	J/mol×K	1040.33	Joback Method
cpg	711.87	J/mol×K	1080.00	Joback Method

cpg	716.92	J/mol×K	1119.67	Joback Method
cpg	721.07	J/mol×K	1159.34	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=C77207013&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