

Methyl 5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nitrobenzoate

Other names:	Methyl 5-[2-chloro-5-(trifluoromethyl)phenoxy]-2-nitrobenzoate
Inchi:	InChI=1S/C15H9ClF3NO5/c1-24-14(21)10-7-9(3-5-12(10)20(22)23)25-13-6-8(15(17,18)19)
InchiKey:	QBFYBNCGOQKESJ-UHFFFAOYSA-N
Formula:	C15H9ClF3NO5
SMILES:	<chem>COC(=O)c1cc(Oc2cc(C(F)(F)F)ccc2Cl)ccc1[N+](=O)[O-]</chem>
Mol. weight [g/mol]:	375.68
CAS:	121325-44-8

Physical Properties

Property code	Value	Unit	Source
gf	-635.17	kJ/mol	Joback Method
hf	-926.35	kJ/mol	Joback Method
hfus	42.49	kJ/mol	Joback Method
hvap	84.98	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	4.846		Crippen Method
mcvol	222.970	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	2247.00		NIST Webbook
tb	898.44	K	Joback Method
tc	1139.12	K	Joback Method
tf	633.84	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.81	J/molxK	898.44	Joback Method
cpg	635.67	J/molxK	938.55	Joback Method
cpg	643.46	J/molxK	978.67	Joback Method
cpg	650.22	J/molxK	1018.78	Joback Method
cpg	655.99	J/molxK	1058.89	Joback Method
cpg	660.82	J/molxK	1099.00	Joback Method
cpg	664.75	J/molxK	1139.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C121325448&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvpap:	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
rinppl:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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