3-(3-[Trifluoromethyl]phenoxy)benzaldehyde

Other names: Benzaldehyde, 3-[3-(trifluoromethyl)phenoxy]-
3-(3'-trifluoromethyl)phenoxy)benzaldehyde
Inchi: InChI=1S/C14H9F3O2/c15-14(16,17)11-4-2-6-13(8-11)19-12-5-1-3-10(7-12)9-18/h1-9H
InchiKey: RPORRWJOHNQOHN-UHFFFAOYSA-N
Formula: C14H9F3O2
SMILES: O=Cc1cccc(Oc2cccc(C(F)(F)F)c2)c1
Mol. weight [g/mol]: 266.22
CAS: 78725-46-9

Physical Properties

Property code	Value	Unit	Source
gf	-513.55	kJ/mol	Joback Method
hf	-697.05	kJ/mol	Joback Method
hfus	24.62	kJ/mol	Joback Method
hvap	58.02	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	4.310		Crippen Method
mcvol	173.350	ml/mol	McGowan Method
pc	2527.73	kPa	Joback Method
tb	648.70	K	Joback Method
tc	868.89	K	Joback Method
tf	393.84	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.13	J/mol×K	648.70	Joback Method
cpg	455.16	J/mol×K	685.40	Joback Method
cpg	467.16	J/mol×K	722.10	Joback Method
cpg	478.18	J/mol×K	758.80	Joback Method
cpg	488.29	J/mol×K	795.50	Joback Method
cpg	497.54	J/mol×K	832.20	Joback Method
cpg	505.99	J/mol×K	868.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78725469&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume