

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

Physical Properties

Property code	Value	Unit	Source
hf	-742.02	kJ/mol	Cheméo Relay (1.0)
hfus	24.62	kJ/mol	Joback Method
hvap	79.41	kJ/mol	Cheméo Relay (1.0)
ie	8.82	eV	Cheméo Relay (1.0)
logp	4.310		Crippen Method
mcvol	173.350	ml/mol	McGowan Method
tb	587.52	K	Cheméo Relay (1.0)
tf	337.17	K	Cheméo Relay (1.0)

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78725469&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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