3,5-Bis(trifluoromethyl)benzaldehyde

Other names: 3,5-di(Trifluoromethyl)benzaldehyde
Inchi: InChI=1S/C9H4F6O/c10-8(11,12)6-1-5(4-16)2-7(3-6)9(13,14)15/h1-4H
InchiKey: LDWLIXZSDPXYDR-UHFFFAOYSA-N
Formula: C9H4F6O
SMILES: O=Cc1cc(C(F)(F)F)cc(C(F)(F)F)c1
Mol. weight [g/mol]: 242.12
CAS: 401-95-6

Physical Properties

Property code	Value	Unit	Source
ea	1.27 ± 0.09	eV	NIST Webbook
ea	1.23 ± 0.09	eV	NIST Webbook
gf	-1144.65	kJ/mol	Joback Method
hf	-1295.24	kJ/mol	Joback Method
hfus	18.27	kJ/mol	Joback Method
hvap	38.45	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.537		Crippen Method
mcvol	126.100	ml/mol	McGowan Method
pc	2659.77	kPa	Joback Method
tb	479.78	K	Joback Method
tc	658.55	K	Joback Method
tf	293.03	K	Joback Method
vc	0.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.53	J/mol×K	479.78	Joback Method
cpg	301.95	J/mol×K	509.58	Joback Method
cpg	311.62	J/mol×K	539.37	Joback Method
cpg	320.58	J/mol×K	569.17	Joback Method
cpg	328.88	J/mol×K	598.96	Joback Method
cpg	336.55	J/mol×K	628.76	Joback Method

cpg	343.63	J/mol×K	658.55	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=C401956&Units=SI

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
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