Benzaldehyde, 4-(trifluoromethyl)-

Other names:	«alpha»,«alpha»,«alpha»-Trifluoro-p-tolualdehyde
	4-Trifluoromethylbenzaldehyde
	p-Trifluoromethylbenzaldehyde
	p-CF3C6H4CHO
Inchi:	InChI=1S/C8H5F3O/c9-8(10,11)7-3-1-6(5-12)2-4-7/h1-5H
InchiKey:	BEOBZEOPTQQELP-UHFFFAOYSA-N
Formula:	C8H5F3O
SMILES:	O=Cc1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]:	174.12
CAS:	455-19-6

Physical Properties

Property code	Value	Unit	Source
affp	805.60	kJ/mol	NIST Webbook
basg	773.80	kJ/mol	NIST Webbook
ea	0.97 ± 0.09	eV	NIST Webbook
ea	0.94 ± 0.09	eV	NIST Webbook
gf	-561.85	kJ/mol	Joback Method
hf	-666.05	kJ/mol	Joback Method
hfus	14.24	kJ/mol	Joback Method
hvap	39.31	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.518		Crippen Method
mcvol	106.700	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
tb	457.34	K	Joback Method
tc	654.26	K	Joback Method
tf	265.05	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.36	J/mol×K	457.34	Joback Method

cpg	232.79	J/mol×K	490.16	Joback Method
cpg	242.49	J/mol×K	522.98	Joback Method
cpg	251.50	J/mol×K	555.80	Joback Method
cpg	259.86	J/mol×K	588.62	Joback Method
cpg	267.59	J/mol×K	621.44	Joback Method
cpg	274.75	J/mol×K	654.26	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	339.70	K	1.70	NIST Webbook
tbrp	353.50 ± 0.50	K	3.30	NIST Webbook

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=C455196&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume