

Benzaldehyde, 2-(trifluoromethyl)-

Other names:	o-Tolualdehyde, «alpha», «alpha», «alpha»-trifluoro-o-(Trifluoromethyl)benzaldehyde 2-(Trifluoromethyl)benzaldehyde «alpha», «alpha», «alpha»-Trifluoro-o-tolualdehyde
Inchi:	InChI=1S/C8H5F3O/c9-8(10,11)7-4-2-1-3-6(7)5-12/h1-5H
InchiKey:	ZDVRPKUWYQVVDX-UHFFFAOYSA-N
Formula:	C8H5F3O
SMILES:	O=Cc1ccccc1C(F)(F)F
Mol. weight [g/mol]:	174.12
CAS:	447-61-0

Physical Properties

Property code	Value	Unit	Source
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/molxK	457.34	Joback Method
cpg	232.79	J/molxK	490.16	Joback Method
cpg	242.49	J/molxK	522.98	Joback Method
cpg	251.50	J/molxK	555.80	Joback Method
cpg	259.86	J/molxK	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	343.50 ± 0.50	K	2.00	NIST Webbook

Sources

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=C447610&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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