2,4,5-Trifluorobenzaldehyde

Other names: Benzaldehyde, 2,4,5-trifluoro-
2,4,5-trifluorobenzaldeide
Inchi: InChI=1S/C7H3F3O/c8-5-2-7(10)6(9)1-4(5)3-11/h1-3H
InchiKey: CYIFJRXFYSUBFW-UHFFFAOYSA-N
Formula: C7H3F3O
SMILES: O=Cc1cc(F)c(F)cc1F
Mol. weight [g/mol]: 160.09
CAS: 165047-24-5

Physical Properties

Property code	Value	Unit	Source
gf	-592.37	kJ/mol	Joback Method
hf	-659.60	kJ/mol	Joback Method
hfus	18.29	kJ/mol	Joback Method
hvap	39.71	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	1.916		Crippen Method
mcvol	92.610	ml/mol	McGowan Method
pc	3607.21	kPa	Joback Method
tb	447.65	K	Joback Method
tc	636.98	K	Joback Method
tf	276.40	K	Joback Method
vc	0.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.21	J/mol×K	447.65	Joback Method
cpg	188.57	J/mol×K	479.21	Joback Method
cpg	195.57	J/mol×K	510.76	Joback Method
cpg	202.23	J/mol×K	542.32	Joback Method
cpg	208.56	J/mol×K	573.87	Joback Method
cpg	214.56	J/mol×K	605.43	Joback Method
cpg	220.24	J/mol×K	636.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C165047245&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