Benzaldehyde, 4-(trifluoromethoxy)-

Other names: p-(trifluoromethoxy)benzaldehyde
Inchi: InChI=1S/C8H5F3O2/c9-8(10,11)13-7-3-1-6(5-12)2-4-7/h1-5H
InchiKey: XQNVDQZWOBPLQZ-UHFFFAOYSA-N
Formula: C8H5F3O2
SMILES: O=Cc1ccc(OC(F)(F)F)cc1
Mol. weight [g/mol]: 190.12
CAS: 659-28-9

Physical Properties

Property code	Value	Unit	Source
gf	-666.85	kJ/mol	Joback Method
hf	-798.27	kJ/mol	Joback Method
hfus	15.43	kJ/mol	Joback Method
hvap	41.72	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.398		Crippen Method
mcvol	112.570	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
tb	479.76	K	Joback Method
tc	675.46	K	Joback Method
tf	287.28	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.24	J/mol×K	479.76	Joback Method
cpg	254.32	J/mol×K	512.38	Joback Method
cpg	263.76	J/mol×K	544.99	Joback Method
cpg	272.59	J/mol×K	577.61	Joback Method
cpg	280.83	J/mol×K	610.23	Joback Method
cpg	288.51	J/mol×K	642.85	Joback Method
cpg	295.64	J/mol×K	675.46	Joback Method

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=C659289&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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