

4-(Trifluoromethoxy)benzaldehyde

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

Physical Properties

Property code	Value	Unit	Source
hfus	15.43	kJ/mol	Joback Method
hvap	51.07	kJ/mol	Cheméo Relay (1.0)
ie	9.81	eV	Cheméo Relay (1.0)
log10ws	-2.54		Cheméo Relay (1.0)
logp	2.398		Crippen Method
mcvol	112.570	ml/mol	McGowan Method
tb	454.33	K	Cheméo Relay (1.0)
tc	633.67	K	Cheméo Relay (1.0)
tf	256.75	K	Cheméo Relay (1.0)

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C659289&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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