

2-Fluoro-3-(trifluoromethyl)benzoic acid

Inchi:	InChI=1S/C8H4F4O2/c9-6-4(7(13)14)2-1-3-5(6)8(10,11)12/h1-3H,(H,13,14)
InchiKey:	XVEAMDNSCPPPCP-UHFFFAOYSA-N
Formula:	C8H4F4O2
SMILES:	O=C(O)c1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]:	208.11
CAS:	115029-22-6

Physical Properties

Property code	Value	Unit	Source
gf	-932.51	kJ/mol	Joback Method
hf	-1052.86	kJ/mol	Joback Method
hfus	20.33	kJ/mol	Joback Method
hvap	55.86	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.543		Crippen Method
mcvol	114.340	ml/mol	McGowan Method
pc	3497.14	kPa	Joback Method
tb	558.98	K	Joback Method
tc	741.94	K	Joback Method
tf	346.91	K	Joback Method
vc	0.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.03	J/molxK	558.98	Joback Method
cpg	279.89	J/molxK	589.47	Joback Method
cpg	287.21	J/molxK	619.97	Joback Method
cpg	294.04	J/molxK	650.46	Joback Method
cpg	300.39	J/molxK	680.95	Joback Method
cpg	306.29	J/molxK	711.45	Joback Method
cpg	311.77	J/molxK	741.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C115029226&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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