2-Fluoro-3-(trifluoromethyl)phenol, methyl ether

Inchi: InChI=1S/C8H6F4O/c1-13-6-4-2-3-5(7(6)9)8(10,11)12/h2-4H,1H3
InchiKey: YZZDEYSCSPZMIG-UHFFFAOYSA-N
Formula: C8H6F4O
SMILES: COc1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]: 194.13

Physical Properties

Property code	Value	Unit	Source
gf	-771.77	kJ/mol	Joback Method
hf	-920.27	kJ/mol	Joback Method
hfus	15.83	kJ/mol	Joback Method
hvap	34.85	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.853		Crippen Method
mcvol	112.770	ml/mol	McGowan Method
pc	2881.21	kPa	Joback Method
rinpol	997.30		NIST Webbook
rinpol	997.30		NIST Webbook
tb	435.35	K	Joback Method
tc	616.72	K	Joback Method
tf	258.39	K	Joback Method
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	235.63	J/mol×K	435.35	Joback Method
cpg	246.04	J/mol×K	465.58	Joback Method
cpg	255.90	J/mol×K	495.81	Joback Method
cpg	265.24	J/mol×K	526.03	Joback Method
cpg	274.08	J/mol×K	556.26	Joback Method
cpg	282.41	J/mol×K	586.49	Joback Method
cpg	290.28	J/mol×K	616.72	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352578&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume