2-Fluoro-3-(trifluoromethyl)phenol

Inchi: InChI=1S/C7H4F4O/c8-6-4(7(9,10)11)2-1-3-5(6)12/h1-3,12H
InchiKey: DOICLFHNNMXINV-UHFFFAOYSA-N
Formula: C7H4F4O
SMILES: Oc1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]: 180.10
CAS: 207291-85-8

Physical Properties

Property code	Value	Unit	Source
gf	-820.18	kJ/mol	Joback Method
hf	-933.25	kJ/mol	Joback Method
hfus	18.23	kJ/mol	Joback Method
hvap	42.56	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.550		Crippen Method
mcvol	98.680	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
rinpol	954.80		NIST Webbook
tb	465.69	K	Joback Method
tc	664.06	K	Joback Method
tf	324.09	K	Joback Method
vc	0.346	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.03	J/mol×K	465.69	Joback Method
cpg	230.34	J/mol×K	498.75	Joback Method
cpg	238.84	J/mol×K	531.81	Joback Method
cpg	246.62	J/mol×K	564.88	Joback Method
cpg	253.72	J/mol×K	597.94	Joback Method
cpg	260.22	J/mol×K	631.00	Joback Method
cpg	266.17	J/mol×K	664.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C207291858&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume