2-Fluoro-4-(trifluoromethyl)benzoic acid

Inchi: InChI=1S/C8H4F4O2/c9-6-3-4(8(10,11)12)1-2-5(6)7(13)14/h1-3H,(H,13,14)
InchiKey: OCIYTBZXTFPSPI-UHFFFAOYSA-N
Formula: C8H4F4O2
SMILES: O=C(O)c1ccc(C(F)(F)F)cc1F
Mol. weight [g/mol]: 208.11
CAS: 115029-24-8

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/mol×K	558.98	Joback Method
cpg	279.89	J/mol×K	589.47	Joback Method
cpg	287.21	J/mol×K	619.97	Joback Method
cpg	294.04	J/mol×K	650.46	Joback Method
cpg	300.39	J/mol×K	680.95	Joback Method
cpg	306.29	J/mol×K	711.45	Joback Method
cpg	311.77	J/mol×K	741.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C115029248&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

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