2-Fluoro-3-(trifluoromethyl)propiophenone

Inchi: InChI=1S/C10H8F4O/c1-2-8(15)6-4-3-5-7(9(6)11)10(12,13)14/h3-5H,2H2,1H3
InchiKey: GUQSGIYHKUPVTH-UHFFFAOYSA-N
Formula: C10H8F4O
SMILES: CCC(=O)c1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]: 220.16
CAS: 207986-23-0

Physical Properties

Property code	Value	Unit	Source
gf	-778.85	kJ/mol	Joback Method
hf	-941.91	kJ/mol	Joback Method
hfus	21.42	kJ/mol	Joback Method
hvap	43.64	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.437		Crippen Method
mcvol	136.650	ml/mol	McGowan Method
pc	2563.69	kPa	Joback Method
tb	512.56	K	Joback Method
tc	701.16	K	Joback Method
tf	308.63	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.15	J/mol×K	512.56	Joback Method
cpg	324.79	J/mol×K	543.99	Joback Method
cpg	335.71	J/mol×K	575.43	Joback Method
cpg	345.96	J/mol×K	606.86	Joback Method
cpg	355.55	J/mol×K	638.29	Joback Method
cpg	364.53	J/mol×K	669.73	Joback Method
cpg	372.92	J/mol×K	701.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C207986230&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

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