2-Fluoro-5-(trifluoromethyl)benzophenone

Inchi: InChI=1S/C14H8F4O/c15-12-7-6-10(14(16,17)18)8-11(12)13(19)9-4-2-1-3-5-9/h1-8H
InchiKey: SRXSIASKXYCRCC-UHFFFAOYSA-N
Formula: C14H8F4O
SMILES: O=C(c1ccccc1)c1cc(C(F)(F)F)ccc1F
Mol. weight [g/mol]: 268.21
CAS: 199292-40-5

Physical Properties

Property code	Value	Unit	Source
gf	-632.76	kJ/mol	Joback Method
hf	-787.94	kJ/mol	Joback Method
hfus	25.82	kJ/mol	Joback Method
hvap	54.82	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	4.075		Crippen Method
mcvol	169.250	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
tb	630.76	K	Joback Method
tc	848.27	K	Joback Method
tf	380.13	K	Joback Method
vc	0.670	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.04	J/mol×K	630.76	Joback Method
cpg	438.06	J/mol×K	667.01	Joback Method
cpg	450.03	J/mol×K	703.26	Joback Method
cpg	461.02	J/mol×K	739.52	Joback Method
cpg	471.09	J/mol×K	775.77	Joback Method
cpg	480.32	J/mol×K	812.02	Joback Method
cpg	488.77	J/mol×K	848.27	Joback Method

Sources

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=C199292405&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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