2-(Trifluoromethyl)benzophenone

Other names: o-Trifluoromethylbenzophenone
Methanone, phenyl[2-(trifluoromethyl)phenyl]-
Inchi: InChI=1S/C14H9F3O/c15-14(16,17)12-9-5-4-8-11(12)13(18)10-6-2-1-3-7-10/h1-9H
InchiKey: JXIWJBWMQXDALU-UHFFFAOYSA-N
Formula: C14H9F3O
SMILES: O=C(c1ccccc1)c1ccccc1C(F)(F)F
Mol. weight [g/mol]: 250.22
CAS: 727-99-1

Physical Properties

Property code	Value	Unit	Source
gf	-428.32	kJ/mol	Joback Method
hf	-580.36	kJ/mol	Joback Method
hfus	23.13	kJ/mol	Joback Method
hvap	54.97	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.936		Crippen Method
mcvol	167.480	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
tb	626.51	K	Joback Method
tc	853.58	K	Joback Method
tf	367.02	K	Joback Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.80	J/mol×K	626.51	Joback Method
cpg	431.75	J/mol×K	664.36	Joback Method
cpg	444.51	J/mol×K	702.20	Joback Method
cpg	456.17	J/mol×K	740.05	Joback Method
cpg	466.81	J/mol×K	777.89	Joback Method
cpg	476.52	J/mol×K	815.74	Joback Method
cpg	485.37	J/mol×K	853.58	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=C727991&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