3'-(Trifluoromethyl)acetophenone

Other names:	3-Trifluoromethylacetophenone
	m-Trifluoromethylacetophenone
	3-Trifludromethylacetophenone
	Ethanone, 1-[3-(trifluoromethyl)phenyl]-
	3-CF3-C6H4-COCH3
Inchi:	InChI=1S/C9H7F3O/c1-6(13)7-3-2-4-8(5-7)9(10,11)12/h2-5H,1H3
InchiKey:	ABXGMGUHGLQMAW-UHFFFAOYSA-N
Formula:	C9H7F3O
SMILES:	CC(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	188.15
CAS:	349-76-8

Physical Properties

Property code	Value	Unit	Source
affp	835.60	kJ/mol	NIST Webbook
basg	803.70	kJ/mol	NIST Webbook
ea	0.66 ± 0.01	eV	NIST Webbook
ea	0.77 ± 0.09	eV	NIST Webbook
gf	-582.83	kJ/mol	Joback Method
hf	-713.69	kJ/mol	Joback Method
hfus	16.14	kJ/mol	Joback Method
hvap	41.56	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.908		Crippen Method
mcvol	120.790	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
tb	472.00 ± 1.00	K	NIST Webbook
tc	685.09	K	Joback Method
tf	284.25	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	261.80	J/mol×K	485.43	Joback Method
cpg	273.51	J/mol×K	518.71	Joback Method
cpg	284.43	J/mol×K	551.98	Joback Method
cpg	294.60	J/mol×K	585.26	Joback Method
cpg	304.05	J/mol×K	618.54	Joback Method
cpg	312.82	J/mol×K	651.81	Joback Method
cpg	320.96	J/mol×K	685.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C349768&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

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
ea:	Electron affinity
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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