2'-(Trifluoromethyl)acetophenone

Other names:	o-Trifluoromethylacetophenone
	2-Trifluoromethylacetophenone
	Ethanone, 1-[2-(trifluoromethyl)phenyl]-
	Acetophenone, 2'-trifluoromethyl-
Inchi:	InChI=1S/C9H7F3O/c1-6(13)7-4-2-3-5-8(7)9(10,11)12/h2-5H,1H3
InchiKey:	FYDUUODXZQITBF-UHFFFAOYSA-N
Formula:	C9H7F3O
SMILES:	CC(=O)c1ccccc1C(F)(F)F
Mol. weight [g/mol]:	188.15
CAS:	17408-14-9

Physical Properties

Property code	Value	Unit	Source
ea	0.64 ± 0.01	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	485.43	K	Joback Method
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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	364.00	K	1.60	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17408149&Units=SI

Legend

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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume