4'-(TRIFLUOROMETHYL)ACETOPHENONE

Other names:	p-Trifluoromethylacetophenone
	4-Trifluoromethylacetophenone
	Ethanone, 1-[4-(trifluoromethyl)phenyl]-
	4-CF3-C6H4-COCH3
	1-[4-(trifluoromethyl)phenyl]ethan-1-one
Inchi:	InChI=1S/C9H7F3O/c1-6(13)7-2-4-8(5-3-7)9(10,11)12/h2-5H,1H3
InchiKey:	HHAISVSEJFEWBZ-UHFFFAOYSA-N
Formula:	C9H7F3O
SMILES:	CC(=O)c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]:	188.15

Physical Properties

Property code	Value	Unit	Source
af	0.4353		Cheméo Relay (1.0)
affp	836.90	kJ/mol	NIST Webbook
basg	805.00	kJ/mol	NIST Webbook
ea	0.90 ± 0.09	eV	NIST Webbook
ea	0.85 ± 0.09	eV	NIST Webbook
ea	0.64 ± 0.01	eV	NIST Webbook
gf	-582.83	kJ/mol	Joback Method
hf	-776.18	kJ/mol	Cheméo Relay (1.0)
hfus	16.14	kJ/mol	Joback Method
hvap	59.79	kJ/mol	Cheméo Relay (1.0)
ie	9.97	eV	Cheméo Relay (1.0)
log10ws	-2.43		Cheméo Relay (1.0)
logp	2.908		Crippen Method
mcvol	120.790	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
tb	464.62	K	Cheméo Relay (1.0)
tc	662.14	K	Cheméo Relay (1.0)
tf	329.61	K	Cheméo Relay (1.0)
vc	0.442	m3/kmol	Cheméo Relay (1.0)

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	355.50 ± 1.50	K	1.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C709637&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
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
ie:	Ionization energy
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

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