(M-(TRIFLUOROMETHYL)PHENYL)ACETONE

Other names:	2-Propanone, 1-(«alpha»,«alpha»,«alpha»-trifluoro-m-tolyl)-
	m-(Trifluoromethyl)benzyl methyl ketone
	m-Trifluoromethylphenylacetone
	[3-(Trifluoromethyl)phenyl]acetone
	1-(3-Trifluoromethylphenyl)-2-propanone
	1-(«alpha»,«alpha»,«alpha»-Trifluoro-m-tolyl)-2-propanone
	1-(«alpha»,«alpha»,«alpha»-trifluoro-m-tolyl)acetone
Inchi:	InChI=1S/C10H9F3O/c1-7(14)5-8-3-2-4-9(6-8)10(11,12)13/h2-4,6H,5H2,1H3
InchiKey:	JPHQCDCEBDRIOL-UHFFFAOYSA-N
Formula:	C10H9F3O
SMILES:	CC(=O)Cc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	202.18

Physical Properties

Property code	Value	Unit	Source
hf	-776.75	kJ/mol	Cheméo Relay (1.0)
hfus	18.73	kJ/mol	Joback Method
hvap	54.44	kJ/mol	Cheméo Relay (1.0)
ie	9.29	eV	Cheméo Relay (1.0)
log10ws	-1.92		Cheméo Relay (1.0)
logp	2.837		Crippen Method
mcvol	134.880	ml/mol	McGowan Method
tb	481.42	K	Cheméo Relay (1.0)
tf	305.42	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.82	J/mol×K	508.31	Joback Method
cpg	317.42	J/mol×K	541.15	Joback Method
cpg	329.18	J/mol×K	573.99	Joback Method
cpg	340.17	J/mol×K	606.83	Joback Method
cpg	350.41	J/mol×K	639.67	Joback Method
cpg	359.95	J/mol×K	672.51	Joback Method

cpg	368.83	J/mol×K	705.35	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	362.70	K	0.07	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21906398&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point