2-Propanone, 1-[3-(trifluoromethyl)phenyl]-

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]: 202.17
CAS: 21906-39-8

Physical Properties

Property code	Value	Unit	Source
gf	-574.41	kJ/mol	Joback Method
hf	-734.33	kJ/mol	Joback Method
hfus	18.73	kJ/mol	Joback Method
hvap	43.79	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.837		Crippen Method
mcvol	134.880	ml/mol	McGowan Method
pc	2726.86	kPa	Joback Method
tb	508.31	K	Joback Method
tc	705.35	K	Joback Method
tf	295.52	K	Joback Method
vc	0.536	m3/kmol	Joback Method

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21906398&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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