3-(Trifluoromethyl)propiophenone

Other names: 3-(Trifluoromethyl)propiophenone
Inchi: InChI=1S/C10H9F3O/c1-2-9(14)7-4-3-5-8(6-7)10(11,12)13/h3-6H,2H2,1H3
InchiKey: UBTPNKXHYILGJU-UHFFFAOYSA-N
Formula: C10H9F3O
SMILES: CCC(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 202.18

Physical Properties

Property code	Value	Unit	Source
hf	-792.11	kJ/mol	Cheméo Relay (1.0)
hfus	18.73	kJ/mol	Joback Method
hvap	59.57	kJ/mol	Cheméo Relay (1.0)
ie	9.71	eV	Cheméo Relay (1.0)
log10ws	-2.91		Cheméo Relay (1.0)
logp	3.298		Crippen Method
mcvol	134.880	ml/mol	McGowan Method
tb	479.15	K	Cheméo Relay (1.0)
tf	310.82	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	345.50 ± 0.50	K	0.70	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=C1533035&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

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