

2-(Trifluoromethyl)propiophenone

Other names:	1-[2-(Trifluoromethyl)phenyl]-1-propanone 2-(Trifluoromethyl)propiophenone
Inchi:	InChI=1S/C10H9F3O/c1-2-9(14)7-5-3-4-6-8(7)10(11,12)13/h3-6H,2H2,1H3
InchiKey:	PUSBIOFSWWHNDU-UHFFFAOYSA-N
Formula:	C10H9F3O
SMILES:	CCC(=O)c1ccccc1C(F)(F)F
Mol. weight [g/mol]:	202.18

Physical Properties

Property code	Value	Unit	Source
hfus	18.73	kJ/mol	Joback Method
ie	9.61	eV	Cheméo Relay (1.0)
log10ws	-2.62		Cheméo Relay (1.0)
logp	3.298		Crippen Method
mcvol	134.880	ml/mol	McGowan Method
tb	474.96	K	Cheméo Relay (1.0)
tf	272.74	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	393.00	K	2.70	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C16185969&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

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion 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

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