3'-Trifluoromethylformanilide

Other names: 3'-Trifluoromethylformanilide
Formamide, N-[3-(trifluoromethyl)phenyl]-
Formanilide, 3'-trifluoromethyl-
N-(3-Trifluoromethylphenyl)formamide
N-(«alpha»,«alpha»,«alpha»-Trifluoro-m-tolyl)formamide
m-Formotoluidide, «alpha»,«alpha»,«alpha»-trifluoro-
Inchi: InChI=1S/C8H6F3NO/c9-8(10,11)6-2-1-3-7(4-6)12-5-13/h1-5H,(H,12,13)
InchiKey: PPECHNDWLRNHEA-UHFFFAOYSA-N
Formula: C8H6F3NO
SMILES: O=CNc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 189.14

Physical Properties

Property code	Value	Unit	Source
hf	-702.77	kJ/mol	Cheméo Relay (1.0)
hfus	19.34	kJ/mol	Joback Method
hvap	65.67	kJ/mol	Cheméo Relay (1.0)
ie	9.28	eV	Cheméo Relay (1.0)
log10ws	-2.20		Cheméo Relay (1.0)
logp	2.274		Crippen Method
mcvol	116.680	ml/mol	McGowan Method
tb	500.36	K	Cheméo Relay (1.0)
tf	326.80	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.32	J/mol×K	507.51	Joback Method
cpg	274.87	J/mol×K	540.67	Joback Method
cpg	284.66	J/mol×K	573.82	Joback Method
cpg	293.74	J/mol×K	606.98	Joback Method
cpg	302.15	J/mol×K	640.13	Joback Method
cpg	309.91	J/mol×K	673.29	Joback Method
cpg	317.08	J/mol×K	706.45	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C657783&Units=SI
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
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
tf:	Normal melting (fusion) point