4-(Trifluoromethyl)benzamide

Other names:	p-Trifluoromethylbenzamide
	N-(4-Trifluoromethyl)benzamide
	Benzamide, 4-(trifluoromethyl)-
	4-CF3-C6H4CONH2
Inchi:	InChI=1S/C8H6F3NO/c9-8(10,11)6-3-1-5(2-4-6)7(12)13/h1-4H,(H2,12,13)
InchiKey:	WEJHBEDHLLBJFW-UHFFFAOYSA-N
Formula:	C8H6F3NO
SMILES:	NC(=O)c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]:	189.13
CAS:	1891-90-3

Physical Properties

Property code	Value	Unit	Source
affp	862.80	kJ/mol	NIST Webbook
basg	831.80	kJ/mol	NIST Webbook
gf	-524.80	kJ/mol	Joback Method
hf	-659.26	kJ/mol	Joback Method
hfus	18.75	kJ/mol	Joback Method
hvap	49.98	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	1.804		Crippen Method
mcvol	116.680	ml/mol	McGowan Method
pc	3602.88	kPa	Joback Method
tb	535.08	K	Joback Method
tc	748.18	K	Joback Method
tf	356.24	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.67	J/mol×K	535.08	Joback Method
cpg	282.12	J/mol×K	570.60	Joback Method
cpg	291.77	J/mol×K	606.11	Joback Method

cpg	300.65	J/mol×K	641.63	Joback Method
cpg	308.81	J/mol×K	677.15	Joback Method
cpg	316.31	J/mol×K	712.67	Joback Method
cpg	323.18	J/mol×K	748.18	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1891903&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

affp: Proton affinity
basg: Gas basicity
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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume