m-Toluamide

Other names: 3-methylbenzamide
Benzamide, 3-methyl-
m-methylbenzamide
Inchi: InChI=1S/C8H9NO/c1-6-3-2-4-7(5-6)8(9)10/h2-5H,1H3,(H2,9,10)
InchiKey: WGRPQCFFBRDZFV-UHFFFAOYSA-N
Formula: C8H9NO
SMILES: Cc1cccc(C(N)=O)c1
Mol. weight [g/mol]: 135.16
CAS: 618-47-3

Physical Properties

Property code	Value	Unit	Source
affp	900.90	kJ/mol	NIST Webbook
basg	869.90	kJ/mol	NIST Webbook
gf	56.79	kJ/mol	Joback Method
hf	-62.18	kJ/mol	Joback Method
hfus	21.60	kJ/mol	Experimental and computational thermodynamic study of ortho-, meta-, and para-methylbenzamide
hvap	53.73	kJ/mol	Joback Method
ie	9.11	eV	NIST Webbook
log10ws	-2.12		Crippen Method
logp	1.094		Crippen Method
mcvol	111.370	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
tb	540.50	K	Joback Method
tc	774.37	K	Joback Method
tf	352.05	K	Joback Method
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	242.96	J/mol×K	540.50	Joback Method
cpg	254.36	J/mol×K	579.48	Joback Method
cpg	265.00	J/mol×K	618.46	Joback Method
cpg	274.92	J/mol×K	657.43	Joback Method
cpg	284.13	J/mol×K	696.41	Joback Method
cpg	292.68	J/mol×K	735.39	Joback Method
cpg	300.60	J/mol×K	774.37	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C618473&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and computational thermodynamic study of ortho-, meta-, and para-methylbenzamide:	https://www.doi.org/10.1016/j.jct.2011.09.024

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
ie:	Ionization energy
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