Benzamide, 2-methyl-

Other names:	2-methylbenzamide
	o-Methylbenzamide
	o-Toluamide
	o-Tolylamide
	o-toluic amide
Inchi:	InChI=1S/C8H9NO/c1-6-4-2-3-5-7(6)8(9)10/h2-5H,1H3,(H2,9,10)
InchiKey:	XXUNIGZDNWWYED-UHFFFAOYSA-N
Formula:	C8H9NO
SMILES:	Cc1ccccc1C(N)=O
Mol. weight [g/mol]:	135.16
CAS:	527-85-5

Physical Properties

Property code	Value	Unit	Source
gf	56.79	kJ/mol	Joback Method
hf	-62.18	kJ/mol	Joback Method
hfus	22.90	kJ/mol	Experimental and computational thermodynamic study of ortho-, meta-, and para-methylbenzamide
hvap	53.73	kJ/mol	Joback Method
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

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
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=C527855&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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