3,4-Dimethylbenzamide

Inchi: InChI=1S/C9H11NO/c1-6-3-4-8(9(10)11)5-7(6)2/h3-5H,1-2H3,(H2,10,11)
InchiKey: INGCXEIJXKQPJH-UHFFFAOYSA-N
Formula: C9H11NO
SMILES: Cc1ccc(C(N)=O)cc1C
Mol. weight [g/mol]: 149.19
CAS: 5580-33-6

Physical Properties

Property code	Value	Unit	Source
gf	55.58	kJ/mol	Joback Method
hf	-94.29	kJ/mol	Joback Method
hfus	19.13	kJ/mol	Joback Method
hvap	56.61	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	1.402		Crippen Method
mcvol	125.460	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
tb	568.36	K	Joback Method
tc	798.81	K	Joback Method
tf	375.84	K	Joback Method
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.46	J/mol×K	568.36	Joback Method
cpg	298.58	J/mol×K	606.77	Joback Method
cpg	309.95	J/mol×K	645.18	Joback Method
cpg	320.60	J/mol×K	683.59	Joback Method
cpg	330.55	J/mol×K	722.00	Joback Method
cpg	339.82	J/mol×K	760.40	Joback Method
cpg	348.45	J/mol×K	798.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5580336&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

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