1,3-dimethyl-1-phenylurea

Inchi: InChI=1S/C9H12N2O/c1-10-9(12)11(2)8-6-4-3-5-7-8/h3-7H,1-2H3,(H,10,12)
InchiKey: ZWOULFZCQXICLZ-UHFFFAOYSA-N
Formula: C9H12N2O
SMILES: CNC(=O)N(C)c1ccccc1
Mol. weight [g/mol]: 164.20
CAS: 938-91-0

Physical Properties

Property code	Value	Unit	Source
chs	-5038.80 ± 5.00	kJ/mol	NIST Webbook
gf	208.56	kJ/mol	Joback Method
hf	15.86	kJ/mol	Joback Method
hfs	-217.80 ± 5.00	kJ/mol	NIST Webbook
hfus	22.83	kJ/mol	Joback Method
hvap	53.13	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	1.462		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
tb	548.48	K	Joback Method
tc	764.08	K	Joback Method
tf	354.65 ± 0.00	K	NIST Webbook
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.50	J/mol×K	548.48	Joback Method
cpg	326.22	J/mol×K	584.41	Joback Method
cpg	339.01	J/mol×K	620.35	Joback Method
cpg	350.93	J/mol×K	656.28	Joback Method
cpg	362.01	J/mol×K	692.21	Joback Method
cpg	372.29	J/mol×K	728.14	Joback Method
cpg	381.83	J/mol×K	764.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C938910&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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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