3-(4-Methoxyphenyl)-1,1-dimethylurea

Other names: N,N-Dimethyl-N'-p-methylphenylurea
Inchi: InChI=1S/C10H14N2O2/c1-12(2)10(13)11-8-4-6-9(14-3)7-5-8/h4-7H,1-3H3,(H,11,13)
InchiKey: LCLYWJDPJMDAQN-UHFFFAOYSA-N
Formula: C10H14N2O2
SMILES: COc1ccc(NC(=O)N(C)C)cc1
Mol. weight [g/mol]: 194.23
CAS: 7160-02-3

Physical Properties

Property code	Value	Unit	Source
gf	102.35	kJ/mol	Joback Method
hf	-148.47	kJ/mol	Joback Method
hfus	26.21	kJ/mol	Joback Method
hvap	58.43	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.789		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3069.34	kPa	Joback Method
tb	598.76	K	Joback Method
tc	809.41	K	Joback Method
tf	398.69	K	Joback Method
vc	0.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.52	J/mol×K	598.76	Joback Method
cpg	397.35	J/mol×K	633.87	Joback Method
cpg	410.34	J/mol×K	668.98	Joback Method
cpg	422.52	J/mol×K	704.09	Joback Method
cpg	433.91	J/mol×K	739.20	Joback Method
cpg	444.53	J/mol×K	774.31	Joback Method
cpg	454.40	J/mol×K	809.41	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7160023&Units=SI

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