Urea, 1-(2'-tert-butylphenyl)-3,3-dimethyl-

Inchi: InChI=1S/C13H20N2O/c1-13(2,3)10-8-6-7-9-11(10)14-12(16)15(4)5/h6-9H,1-5H3,(H,14,1
InchiKey: MKQAHUGZUWALSU-UHFFFAOYSA-N
Formula: C13H20N2O
SMILES: CN(C)C(=O)Nc1ccccc1C(C)(C)C
Mol. weight [g/mol]: 220.31

Physical Properties

Property code	Value	Unit	Source
gf	235.45	kJ/mol	Joback Method
hf	-86.92	kJ/mol	Joback Method
hfus	25.38	kJ/mol	Joback Method
hvap	61.40	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	3.078		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2363.37	kPa	Joback Method
tb	641.75	K	Joback Method
tc	856.28	K	Joback Method
tf	412.69	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.10	J/mol×K	641.75	Joback Method
cpg	527.62	J/mol×K	677.50	Joback Method
cpg	543.02	J/mol×K	713.26	Joback Method
cpg	557.34	J/mol×K	749.01	Joback Method
cpg	570.67	J/mol×K	784.77	Joback Method
cpg	583.08	J/mol×K	820.52	Joback Method
cpg	594.63	J/mol×K	856.28	Joback Method

Sources

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=B6009299&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