Urea, 1-benzyl-1-cyclopropyl-3-methyl-

Inchi: InChI=1S/C12H16N2O/c1-13-12(15)14(11-7-8-11)9-10-5-3-2-4-6-10/h2-6,11H,7-9H2,1H3
InchiKey: IDHFFZMIZRGERY-UHFFFAOYSA-N
Formula: C12H16N2O
SMILES: CNC(=O)N(Cc1ccccc1)C1CC1
Mol. weight [g/mol]: 204.27
CAS: 116502-58-0

Physical Properties

Property code	Value	Unit	Source
gf	294.57	kJ/mol	Joback Method
hf	26.74	kJ/mol	Joback Method
hfus	28.73	kJ/mol	Joback Method
hvap	59.72	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	1.990		Crippen Method
mcvol	166.850	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
tb	623.86	K	Joback Method
tc	843.35	K	Joback Method
tf	404.42	K	Joback Method
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.74	J/mol×K	623.86	Joback Method
cpg	458.82	J/mol×K	660.44	Joback Method
cpg	473.72	J/mol×K	697.02	Joback Method
cpg	487.55	J/mol×K	733.60	Joback Method
cpg	500.37	J/mol×K	770.18	Joback Method
cpg	512.28	J/mol×K	806.76	Joback Method
cpg	523.37	J/mol×K	843.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116502580&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

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