Urea, N-phenyl-N-methyl

Inchi: InChI=1S/C8H10N2O/c1-10(8(9)11)7-5-3-2-4-6-7/h2-6H,1H3,(H2,9,11)
InchiKey: SKAADKSETAYKGL-UHFFFAOYSA-N
Formula: C8H10N2O
SMILES: CN(C(N)=O)c1ccccc1
Mol. weight [g/mol]: 150.18

Physical Properties

Property code	Value	Unit	Source
af	0.5916		Cheméo Relay (1.0)
gf	177.20	kJ/mol	Joback Method
hf	-144.18	kJ/mol	Cheméo Relay (1.0)
hfus	20.33	kJ/mol	Joback Method
hvap	72.76	kJ/mol	Cheméo Relay (1.0)
ie	8.63	eV	Cheméo Relay (1.0)
log10ws	-1.42		Cheméo Relay (1.0)
logp	1.202		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	4233.04	kPa	Joback Method
tb	546.94	K	Cheméo Relay (1.0)
tc	795.41	K	Cheméo Relay (1.0)
tf	336.58	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.02	J/mol×K	547.96	Joback Method
cpg	289.56	J/mol×K	586.12	Joback Method
cpg	301.18	J/mol×K	624.27	Joback Method
cpg	311.92	J/mol×K	662.43	Joback Method
cpg	321.83	J/mol×K	700.59	Joback Method
cpg	330.96	J/mol×K	738.74	Joback Method
cpg	339.37	J/mol×K	776.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C4559879
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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