Urea, phenyl-

Other names:	1-Phenylurea
	Monophenylurea
	N-phenylurea
	NSC 2781
	PC
	Phenylcarbamide
	Stabilisator VH
	Stabilizer VH
	Urea, N-phenyl
	VH
	phenylurea
Inchi:	InChI=1S/C7H8N2O/c8-7(10)9-6-4-2-1-3-5-6/h1-5H,(H3,8,9,10)
InchiKey:	LUBJCRLGQSPQNN-UHFFFAOYSA-N
Formula:	C7H8N2O
SMILES:	NC(=O)Nc1ccccc1
Mol. weight [g/mol]:	136.15
CAS:	64-10-8

Physical Properties

Property code	Value	Unit	Source
chs	-3684.00	kJ/mol	NIST Webbook
chs	-3666.40 ± 2.20	kJ/mol	NIST Webbook
gf	147.39	kJ/mol	Joback Method
hf	23.40	kJ/mol	Joback Method
hfs	-231.50 ± 2.20	kJ/mol	NIST Webbook
hfs	-215.00	kJ/mol	NIST Webbook
hfs	-218.60 ± 2.40	kJ/mol	NIST Webbook
hfus	19.82	kJ/mol	Joback Method
hvap	57.27	kJ/mol	Joback Method
ie	8.55	eV	NIST Webbook
log10ws	-1.67		Crippen Method
logp	1.177		Crippen Method
mcvol	107.260	ml/mol	McGowan Method
pc	4917.69	kPa	Joback Method
tb	511.20	K	NIST Webbook
tc	799.09	K	Joback Method
tf	420.60 ± 0.30	K	NIST Webbook

vc	0.390	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.96	J/mol×K	759.71	Joback Method
cpg	242.67	J/mol×K	562.81	Joback Method
cpg	253.47	J/mol×K	602.19	Joback Method
cpg	263.46	J/mol×K	641.57	Joback Method
cpg	272.68	J/mol×K	680.95	Joback Method
cpg	281.17	J/mol×K	720.33	Joback Method
cpg	296.09	J/mol×K	799.09	Joback Method
hfust	23.68	kJ/mol	420.60	NIST Webbook
hfust	23.68	kJ/mol	420.60	NIST Webbook
hfust	23.68	kJ/mol	420.60	NIST Webbook
hsubt	136.00 ± 6.00	kJ/mol	402.00	NIST Webbook
psub	7.14e-03	kPa	413.60	Phenyl substituted ureas: Evaluation of thermochemical data with complementary experimental and computational methods
psub	6.10e-04	kPa	386.00	Phenyl substituted ureas: Evaluation of thermochemical data with complementary experimental and computational methods
psub	1.03e-03	kPa	391.70	Phenyl substituted ureas: Evaluation of thermochemical data with complementary experimental and computational methods

psub	1.54e-03	kPa	396.20	Phenyl substituted ureas: Evaluation of thermochemical data with complementary experimental and computational methods	
psub	2.09e-03	kPa	399.50	Phenyl substituted ureas: Evaluation of thermochemical data with complementary experimental and computational methods	
psub	2.75e-03	kPa	402.40	Phenyl substituted ureas: Evaluation of thermochemical data with complementary experimental and computational methods	
psub	3.94e-03	kPa	406.20	Phenyl substituted ureas: Evaluation of thermochemical data with complementary experimental and computational methods	
psub	4.70e-03	kPa	408.30	Phenyl substituted ureas: Evaluation of thermochemical data with complementary experimental and computational methods	
psub	6.07e-03	kPa	411.50	Phenyl substituted ureas: Evaluation of thermochemical data with complementary experimental and computational methods	
sfust	56.30	J/mol×K	420.60	NIST Webbook	

Sources

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=C64108&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Phenyl substituted ureas: Evaluation of thermochemical data with complementary experimental and computational methods:	https://www.doi.org/10.1016/j.jct.2019.01.022

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
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
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
psub:	Sublimation pressure
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume