Urea, heptyl-

Other names:	Heptylurea
	Urea, n-heptyl-
	1-Heptyl urea
Inchi:	InChI=1S/C8H18N2O/c1-2-3-4-5-6-7-10-8(9)11/h2-7H2,1H3,(H3,9,10,11)
InchiKey:	LDNJCDRFTFLQLF-UHFFFAOYSA-N
Formula:	C8H18N2O
SMILES:	CCCCCCCNC(N)=O
Mol. weight [g/mol]:	158.24
CAS:	42955-46-4

Physical Properties

Property code	Value	Unit	Source
gf	43.40	kJ/mol	Joback Method
hf	-233.77	kJ/mol	Joback Method
hfus	28.37	kJ/mol	Joback Method
hvap	57.22	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	1.625		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
tb	559.01	K	Joback Method
tc	747.81	K	Joback Method
tf	365.77	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.17	J/mol×K	559.01	Joback Method
cpg	375.15	J/mol×K	590.48	Joback Method
cpg	387.50	J/mol×K	621.94	Joback Method
cpg	399.25	J/mol×K	653.41	Joback Method
cpg	410.42	J/mol×K	684.87	Joback Method
cpg	421.02	J/mol×K	716.34	Joback Method

cpg	431.07	J/mol×K	747.81	Joback Method
hfust	29.00	kJ/mol	386.10	NIST Webbook
hfust	26.30	kJ/mol	382.20	NIST Webbook

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=C42955464&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
hfust:	Enthalpy of fusion at a given temperature
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