Urea, 1,3-diphenethyl-

Inchi: InChI=1S/C17H20N2O/c20-17(18-13-11-15-7-3-1-4-8-15)19-14-12-16-9-5-2-6-10-16/h1-
InchiKey: VMQLWVGHPWFHEI-UHFFFAOYSA-N
Formula: C17H20N2O
SMILES: O=C(NCCc1ccccc1)NCCc1ccccc1
Mol. weight [g/mol]: 268.35
CAS: 5467-84-5

Physical Properties

Property code	Value	Unit	Source
gf	366.94	kJ/mol	Joback Method
hf	73.21	kJ/mol	Joback Method
hfus	39.66	kJ/mol	Joback Method
hvap	77.61	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	2.771		Crippen Method
mcvol	224.400	ml/mol	McGowan Method
pc	2269.73	kPa	Joback Method
rinpol	2550.90		NIST Webbook
tb	795.93	K	Joback Method
tc	1024.25	K	Joback Method
tf	489.44	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.49	J/mol×K	795.93	Joback Method
cpg	669.46	J/mol×K	833.98	Joback Method
cpg	683.26	J/mol×K	872.04	Joback Method
cpg	695.96	J/mol×K	910.09	Joback Method
cpg	707.66	J/mol×K	948.14	Joback Method
cpg	718.43	J/mol×K	986.20	Joback Method
cpg	728.36	J/mol×K	1024.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5467845&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume