Urea],1,1'-(1,4-cyclohexylenedimethylene)bis[3-m

Inchi: InChI=1S/C12H24N4O2/c1-13-11(17)15-7-9-3-5-10(6-4-9)8-16-12(18)14-2/h9-10H,3-8H2
InchiKey: KVVRJFPRHMHPMK-UHFFFAOYSA-N
Formula: C12H24N4O2
SMILES: CNC(=O)NCC1CCC(CNC(=O)NC)CC1
Mol. weight [g/mol]: 256.34
CAS: 116373-59-2

Physical Properties

Property code	Value	Unit	Source
gf	166.62	kJ/mol	Joback Method
hf	-268.31	kJ/mol	Joback Method
hfus	43.34	kJ/mol	Joback Method
hvap	81.66	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	0.651		Crippen Method
mcvol	212.140	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
tb	797.26	K	Joback Method
tc	1006.88	K	Joback Method
tf	538.64	K	Joback Method
vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.22	J/mol×K	797.26	Joback Method
cpg	697.54	J/mol×K	832.20	Joback Method
cpg	711.71	J/mol×K	867.13	Joback Method
cpg	724.77	J/mol×K	902.07	Joback Method
cpg	736.75	J/mol×K	937.01	Joback Method
cpg	747.70	J/mol×K	971.95	Joback Method
cpg	757.63	J/mol×K	1006.88	Joback Method

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=C116373592&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
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

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