Urea, 1-(2-cyanoethyl)-3-phenyl-

Inchi: InChI=1S/C10H11N3O/c11-7-4-8-12-10(14)13-9-5-2-1-3-6-9/h1-3,5-6H,4,8H2,(H2,12,13,
InchiKey: OAEZUJCBJHUAQW-UHFFFAOYSA-N
Formula: C10H11N3O
SMILES: N#CCCN=C(O)Nc1ccccc1
Mol. weight [g/mol]: 189.21
CAS: 22193-20-0

Physical Properties

Property code	Value	Unit	Source
hf	125.35	kJ/mol	Joback Method
hvap	77.12	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	1.926		Crippen Method
mcvol	150.910	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
tb	775.87	K	Joback Method
tc	998.28	K	Joback Method

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=C22193200&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation 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

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