Urea, 1,3-bis(2-cyanoethyl)-1-nitroso-

Inchi: InChI=1S/C7H9N5O2/c8-3-1-5-10-7(13)12(11-14)6-2-4-9/h1-2,5-6H2,(H,10,13)
InchiKey: UJMHIEGWBATPGL-UHFFFAOYSA-N
Formula: C7H9N5O2
SMILES: N#CCCNC(=O)N(CCC#N)N=O
Mol. weight [g/mol]: 195.18
CAS: 60285-25-8

Physical Properties

Property code	Value	Unit	Source
hf	-17.82	kJ/mol	Joback Method
hvap	76.45	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	0.507		Crippen Method
mcvol	145.330	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
tb	743.60	K	Joback Method
tc	949.52	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C60285258&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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