Noruron

Other names:
(3a«alpha»,4«alpha»,5«alpha»,7«alpha»,7a«alpha»)-1,1-dimethyl-3-(octahydro-4,7-meth
(3aÂ«alphaÂ»,4Â«alphaÂ»,5Â«alphaÂ»,7Â«alphaÂ»,7aÂ«alphaÂ»)-1,1-dimethyl-3-(octa
1-(3a,4,5,6,7,7a-Hexahydro-4,7-methano-5-indanyl)-3,3-dimethylurea
1-(5-(3a,4,5,6,7,7a-Hexahydro-4,7-methanoindanyl))-3,3-dimethylurea
1-(Tetrahydrodicyclopentadienyl)-3,3-dimethylurea
3-(5-(3a,4,5,6,7,7a-Hexahydro-4,6-methanoindanyl))-1,1-dimethylurea
3-(Hexahydro-4,7-methanoindan-5-yl)-1,1-dimethylurea
Asepta Herban
Herban
Hercules 7531
N,N-dimethyl-N'-(octahydro-4,7-methano-1H-inden-5-yl)urea
Narea
Norea
Nores
Urea, 3-(hexahydro-4,7-methanoindan-5-yl)-1,1-dimethyl-, endo,exo-5-
Urea, N,N-dimethyl-N'-(octahydro-4,7-methano-1H-inden-5-yl)-, (3a«alpha»,4«alpha»,5«alpha»,7«alpha»,7a«alpha»)-
Urea, N,N-dimethyl-N'-(octahydro-4,7-methano-1H-inden-5-yl)-, (3aÂ«alphaÂ»,4Â«alphaÂ»,5Â«alphaÂ»,7Â«alphaÂ»,7aÂ«alphaÂ»)-
Urea, N,N-dimethyl-N'-[(3aR,4S,5R,7S,7aR)-octahydro-4,7-methano-1H-inden-5-yl]-, rel-
Isonoruron

Inchi: InChI=1S/C13H22N2O/c1-15(2)13(16)14-12-7-8-6-11(12)10-5-3-4-9(8)10/h8-12H,3-7H2,
InchiKey: YGLMVCVJLXREAK-PZWNZHSQSA-N
Formula: C13H21N2O
SMILES: CN(C)C(=O)NC1CC2CC1C1CCCC21
Mol. weight [g/mol]: 221.32
CAS: 18530-56-8

Physical Properties

Property code	Value	Unit	Source
gf	284.56	kJ/mol	Joback Method
hf	-131.67	kJ/mol	Joback Method
hfus	33.59	kJ/mol	Joback Method
hvap	59.05	kJ/mol	Joback Method
log10ws	-3.01		Aqueous Solubility Prediction Method
log10ws	-3.17		Estimated Solubility Method
logp	2.082		Crippen Method

mcvol	182.980	ml/mol	McGowan Method
pc	2395.87	kPa	Joback Method
rinpol	1960.00		NIST Webbook
rinpol	1941.00		NIST Webbook
rinpol	1941.00		NIST Webbook
tb	628.47	K	Joback Method
tc	838.21	K	Joback Method
tf	441.87 ± 0.20	K	NIST Webbook
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	635.74	J/mol×K	803.25	Joback Method
cpg	547.21	J/mol×K	628.47	Joback Method
cpg	567.38	J/mol×K	663.43	Joback Method
cpg	586.22	J/mol×K	698.38	Joback Method
cpg	603.82	J/mol×K	733.34	Joback Method
cpg	620.30	J/mol×K	768.30	Joback Method
cpg	650.26	J/mol×K	838.21	Joback Method
hfust	21.74	kJ/mol	436.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18530568&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume