Allantoin

Other names:	2,5-Dioxo-4-imidazolidinyl-urea 2,5-Imidazolidinedione, 4-ureido- 5-Ureidohydantoin 5-Ureidohydrantoin AVC/Dienestrolcream Alantan Allantol Cordianine Fancol TOIN Glyoxyldiureid Glyoxyldiureide Glyoxylic diureide Hydantoin, 5-ureido- NSC 7606 Psoralon Sebical Septalan Urea, (2,5-dioxo-4-imidazolidinyl)- Urea, N-(2,5-dioxo-4-imidazolidinyl)-
Inchi:	InChI=1S/C4H6N4O3/c5-3(10)6-1-2(9)8-4(11)7-1/h1H,(H3,5,6,10)(H2,7,8,9,11)
InchiKey:	POJWUDADGALRAB-UHFFFAOYSA-N
Formula:	$C_4H_6N_4O_3$
SMILES:	NC(=O)NC1NC(=O)NC1=O
Mol. weight [g/mol]:	158.12
CAS:	97-59-6

Physical Properties

Property code	Value	Unit	Source
chs	-1708.90	kJ/mol	NIST Webbook
chs	-1714.00 ± 0.67	kJ/mol	NIST Webbook
gf	-23.49	kJ/mol	Joback Method
hf	-290.51	kJ/mol	Joback Method
hfs	-717.56 ± 0.71	kJ/mol	NIST Webbook
hfus	30.15	kJ/mol	Joback Method
hvap	70.59	kJ/mol	Joback Method
log10ws	-1.60		Aqueous Solubility Prediction Method

log10ws	-1.60		Estimated Solubility Method
logp	-2.180		Crippen Method
mcvol	100.990	ml/mol	McGowan Method
pc	7317.64	kPa	Joback Method
ss	195.00	J/mol×K	NIST Webbook
tb	715.51	K	Joback Method
tc	981.00	K	Joback Method
tf	678.09	K	Joback Method
vc	0.358	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.11	J/mol×K	715.51	Joback Method
cpg	292.03	J/mol×K	759.76	Joback Method
cpg	301.97	J/mol×K	804.01	Joback Method
cpg	310.84	J/mol×K	848.26	Joback Method
cpg	318.51	J/mol×K	892.50	Joback Method
cpg	324.90	J/mol×K	936.75	Joback Method
cpg	329.88	J/mol×K	981.00	Joback Method
cps	179.95	J/mol×K	296.60	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C97596&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

Legend

chs: Standard solid enthalpy of combustion

cpg: Ideal gas heat capacity

cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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