

Biotin

Other names:

1H-Thieno[3,4-d]imidazole-4-pentanoic acid, hexahydro-2-oxo-,
[3aS,(3a«alpha»,4«beta»,6a«alpha»)]-
(+)-Biotin
d-Biotin
Bioepiderm
Bios II
Coenzyme R
Factor S
Vitamin B7
Vitamin H
Factor S (vitamin)
Injacom H
D-(+)-Biotin
(3aS,4S,6aR)-Hexahydro-2-oxo-1H-thieno[3,4-d]imidazole-4-valeric acid
Biodermatin
1H-Thieno[3,4-d]imidazole-4-pentanoic acid, hexahydro-2-oxo-, (3aS,4S,6aR)-
NSC 63865

Inchi:

InChI=1S/C10H16N2O3S/c13-8(14)4-2-1-3-7-9-6(5-16-7)11-10(15)12-9/h6-7,9H,1-5H2,(

InchiKey:

YBJHBAHKTYVGT-UHFFFAOYSA-N

Formula:

C10H16N2O3S

SMILES:

O=C(O)CCCC1SCC2NC(=O)NC21

Mol. weight [g/mol]:

244.31

CAS:

58-85-5

Physical Properties

Property code	Value	Unit	Source
gf	-50.14	kJ/mol	Joback Method
hf	-418.42	kJ/mol	Joback Method
hfus	42.83	kJ/mol	Joback Method
hvap	84.71	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	0.797		Crippen Method
mcvol	175.360	ml/mol	McGowan Method
pc	3598.56	kPa	Joback Method
tb	804.35	K	Joback Method
tc	1031.24	K	Joback Method
tf	699.54	K	Joback Method
vc	0.644	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.01	J/mol×K	804.35	Joback Method
cpg	556.20	J/mol×K	842.17	Joback Method
cpg	568.38	J/mol×K	879.98	Joback Method
cpg	579.57	J/mol×K	917.80	Joback Method
cpg	589.77	J/mol×K	955.61	Joback Method
cpg	599.01	J/mol×K	993.43	Joback Method
cpg	607.31	J/mol×K	1031.24	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=C58855&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
mccvol:	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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