Penicillamine

Other names:

(-)-Penicillamine
(2S)-2-Amino-3-methyl-3-sulfanylbutanoic acid
(S)-3,3-Dimethylcysteine
(S)-Penicillamin
(S)-Penicillamine
.beta.,.beta.-dimethylcysteine
2-Amino-3-mercapto-3-methylbutanoic acid
3-sulfanylvaline
Artamine
Cuprenil
Cuprimine
Cupripen
D-(-)-Penicillamine
D-3-Mercaptovaline
D-Mercaptovaline
D-Penamine
D-Penicillamine
D-Valine, 3-mercapto-
D-«beta»,«beta»-Dimethylcysteine
D-«beta»-Thiovaline
D-Â«betaÂ»,Â«betaÂ»-Dimethylcysteine
D-Â«betaÂ»-Thiovaline
DL-3-mercaptovaline
DL-penicillamine
DPA
Depamine
Depen
Kuprenil
Mercaptyl
Metalcaptase
NSC 81549
Pendramine
Penicillamin
Perdolat
Reduced D-penicillamine
Reduced penicillamine
Sufirtan
Trolovol
Valine, 3-mercapto-, D-
pencillamine

	«beta»-Thiovaline
	Â«betaÂ»-Thiovaline
Inchi:	InChI=1S/C5H11NO2S/c1-5(2,9)3(6)4(7)8/h3,9H,6H2,1-2H3,(H,7,8)
InchiKey:	VVNCNSJFMMFHPL-UHFFFAOYSA-N
Formula:	C5H11NO2S
SMILES:	CC(C)(S)C(N)C(=O)O
Mol. weight [g/mol]:	149.21
CAS:	52-67-5

Physical Properties

Property code	Value	Unit	Source
gf	-178.28	kJ/mol	Joback Method
hf	-353.10	kJ/mol	Joback Method
hfus	12.69	kJ/mol	Joback Method
hvap	65.84	kJ/mol	Joback Method
log10ws	-0.13		Aqueous Solubility Prediction Method
logp	0.107		Crippen Method
mcvol	115.080	ml/mol	McGowan Method
pc	5138.68	kPa	Joback Method
tb	591.57	K	Joback Method
tc	808.47	K	Joback Method
tf	471.65	K	Aqueous Solubility Prediction Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.87	J/mol×K	591.57	Joback Method
cpg	285.84	J/mol×K	627.72	Joback Method
cpg	294.17	J/mol×K	663.87	Joback Method
cpg	301.91	J/mol×K	700.02	Joback Method
cpg	309.09	J/mol×K	736.17	Joback Method
cpg	315.76	J/mol×K	772.32	Joback Method
cpg	321.95	J/mol×K	808.47	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Enthalpies of Dilution of Penicillamines in N,N-Dimethylformamide + Water Mixtures at 298.15 K:	https://www.doi.org/10.1021/je300783e
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52675&Units=SI

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume