

Lipoamide

Other names:	1,2-Dithiolane-3-pentanamide 1,2-Dithiolane-3-valeramide Lipamide «alpha»-Lipamide Lipoacin Lipoamid «alpha»-Lipoamide «alpha»-Lipoic acid amide Lipoicin Lipozyme Lypoaran Pathoclon Thioami Thioctamid Thioctamide Thioctic acid amide Thiotomin Ticolin 6-Thioctic acid amide 5-(1,2)Dithiolan-3-yl-pentanoic acid amide 5-(1,2-Dithiolan-3-yl)valeramide Vitamin N DL-6-Thioctic amide
Inchi:	InChI=1S/C8H15NOS2/c9-8(10)4-2-1-3-7-5-6-11-12-7/h7H,1-6H2,(H2,9,10)
InchiKey:	FCCDDURTIUXBY-UHFFFAOYSA-N
Formula:	C8H15NOS2
SMILES:	NC(=O)CCCCC1CCSS1
Mol. weight [g/mol]:	205.34
CAS:	3206-73-3

Physical Properties

Property code	Value	Unit	Source
gf	70.28	kJ/mol	Joback Method
hf	-136.24	kJ/mol	Joback Method
hfus	24.52	kJ/mol	Joback Method
hvap	62.67	kJ/mol	Joback Method

log10ws	-3.15		Crippen Method
logp	2.186		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
rinqol	2148.10		NIST Webbook
tb	619.78	K	Joback Method
tc	858.93	K	Joback Method
tf	490.91	K	Joback Method
vc	0.551	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.75	J/mol×K	619.78	Joback Method
cpg	404.30	J/mol×K	659.64	Joback Method
cpg	417.84	J/mol×K	699.50	Joback Method
cpg	430.43	J/mol×K	739.35	Joback Method
cpg	442.12	J/mol×K	779.21	Joback Method
cpg	452.96	J/mol×K	819.07	Joback Method
cpg	463.00	J/mol×K	858.93	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=C3206733&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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