DL-6-Thioctic amide

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:	FCCDDURTIIUXBY-UHFFFAOYSA-N
Formula:	C8H15NOS2
SMILES:	NC(=O)CCCCC1CCSS1
Mol. weight [g/mol]:	205.35

Physical Properties

Property code	Value	Unit	Source
hfus	24.52	kJ/mol	Joback Method
logp	2.186		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
rinpol	2148.10		NIST Webbook

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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3206733&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices