

Thioctic acid

Other names:	(. +/-)-Lipoic acid 1,2-Dithiolane-3-pentanoic acid, (. +/-)- 1,2-Dithiolane-3-valeric acid, (. +/-)- 1,2-dithiolane-3-pentanoic acid 1,2-dithiolane-3-valeric acid 5-(1,2-Dithiolan-3-yl)valeric acid 5-(1,2-dithiolan-3-yl)pentanoic acid 5-(dithiolan-3-yl)valeric acid DL-1,2-Dithiolan-3-valeriansaeure DL-1,2-Dithiolane 3-valeric acid DL-6-Thioctic acid NSC 628502 NSC 90788 Thioctic acid, dl-form Thioctic acid dl-1,2-Dithiolane-3-pentanoic acid dl-6,8-Thioctic acid dl-Lipoic acid dl-Thioctic acid dl-«alpha»-Lipoic acid «alpha»-Lipoic acid
Inchi:	InChI=1S/C8H14O2S2/c9-8(10)4-2-1-3-7-5-6-11-12-7/h7H,1-6H2,(H,9,10)
InchiKey:	AGBQKNBQESQNJD-UHFFFAOYSA-N
Formula:	C8H14O2S2
SMILES:	O=C(O)CCCC1CCSS1
Mol. weight [g/mol]:	206.33
CAS:	1077-28-7

Physical Properties

Property code	Value	Unit	Source
gf	-132.99	kJ/mol	Joback Method
hf	-322.26	kJ/mol	Joback Method
hfus	23.41	kJ/mol	Joback Method
hvap	68.71	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.785		Crippen Method

mvol	152.860	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
tb	639.43	K	Joback Method
tc	852.77	K	Joback Method
tf	468.47	K	Joback Method
vc	0.541	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.01	J/mol×K	639.43	Joback Method
cpg	395.15	J/mol×K	674.99	Joback Method
cpg	406.53	J/mol×K	710.54	Joback Method
cpg	417.19	J/mol×K	746.10	Joback Method
cpg	427.16	J/mol×K	781.66	Joback Method
cpg	436.49	J/mol×K	817.21	Joback Method
cpg	445.22	J/mol×K	852.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1077287&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of 5-(Dithiolan-3-yl)pentanoic Acid in the Mixed Solvents of Cyclohexane + Ethyl Acetate, Heptane + Ethyl Acetate, and Hexane + Ethyl Acetate:	https://www.doi.org/10.1021/je100048g
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hvp:	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

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