

3,4-DITHIAHEXYL-1,6-DIAMINE

Other names:	Ethanamine, 2,2'-dithiobis- Ethylamine, 2,2'-dithiobis- Becaptan disulfure Bis(«beta»-aminoethyl)disulfide Cysteinamine disulfide Cystinamin Cystineamine Decarboxycystine «beta»,«beta»'-Diaminodiethyl disulfide 2,2'-Dithiobis(ethylamine) 1591 L Mercamine disulfide «beta»-Mercaptoethylamine disulfide 3,4-Dithiahexyl-1,6-diamine 2-Aminoethyl disulfide
Inchi:	InChI=1S/C4H12N2S2/c5-1-3-7-8-4-2-6/h1-6H2
InchiKey:	APQPRKLAWCIJEK-UHFFFAOYSA-N
Formula:	C4H12N2S2
SMILES:	NCCSSCCN
Mol. weight [g/mol]:	152.29

Physical Properties

Property code	Value	Unit	Source
hfus	24.77	kJ/mol	Joback Method
logp	0.285		Crippen Method
mcvol	119.880	ml/mol	McGowan Method
rinpol	1410.00		NIST Webbook
rinpol	1410.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.88	J/mol×K	573.54	Joback Method
cpg	281.36	J/mol×K	613.55	Joback Method

cpg	291.23	J/mol×K	653.57	Joback Method
cpg	300.48	J/mol×K	693.58	Joback Method
cpg	309.10	J/mol×K	733.60	Joback Method
cpg	317.11	J/mol×K	773.61	Joback Method
cpg	324.50	J/mol×K	813.63	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C51854&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>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

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

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