

S-2-[1-ADAMANTYLAMINO]ETHYL THIOSULFURIC ACID

Other names:	2-(1-Adamantyl)aminoethanethiol hydrogen sulfate S-2-[1-Adamantylamino]ethyl thiosulfuric acid 2-(Adamantylamino)ethanethiol, S-hydrogen sulfate
Inchi:	InChI=1S/C12H21NO3S2/c14-18(15,16)17-2-1-13-12-6-9-3-10(7-12)5-11(4-9)8-12/h9-11
InchiKey:	YXDYLGVBKBJRMA-UHFFFAOYSA-N
Formula:	C12H21NO3S2
SMILES:	O=S(=O)(O)SCCNC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	291.44

Physical Properties

Property code	Value	Unit	Source
hfus	38.61	kJ/mol	Joback Method
logp	2.081		Crippen Method
mcpvol	207.650	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.22	J/mol×K	752.93	Joback Method
cpg	658.92	J/mol×K	788.02	Joback Method
cpg	673.94	J/mol×K	823.10	Joback Method
cpg	688.42	J/mol×K	858.19	Joback Method
cpg	702.54	J/mol×K	893.27	Joback Method
cpg	716.44	J/mol×K	928.36	Joback Method
cpg	730.27	J/mol×K	963.44	Joback Method

Sources

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):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C37018318&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Legend

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

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