

THIAZOLIDINE, 2-HEXYL-

Other names:	2-Hexylthiazolidine
Inchi:	InChI=1S/C9H19NS/c1-2-3-4-5-6-9-10-7-8-11-9/h9-10H,2-8H2,1H3
InchiKey:	OAMNFUGALUYNII-UHFFFAOYSA-N
Formula:	C9H19NS
SMILES:	CCCCCCC1NCCS1
Mol. weight [g/mol]:	173.33

Physical Properties

Property code	Value	Unit	Source
hfus	26.25	kJ/mol	Joback Method
logp	2.619		Crippen Method
mcvol	153.140	ml/mol	McGowan Method
rinpol	1402.00		NIST Webbook
rinpol	1402.00		NIST Webbook
tf	293.41	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.60	J/mol×K	516.98	Joback Method
cpg	371.11	J/mol×K	552.17	Joback Method
cpg	387.71	J/mol×K	587.36	Joback Method
cpg	403.43	J/mol×K	622.56	Joback Method
cpg	418.30	J/mol×K	657.75	Joback Method
cpg	432.35	J/mol×K	692.94	Joback Method
cpg	445.61	J/mol×K	728.13	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C40790770&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
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/57-016-1/THIAZOLIDINE-2-HEXYL.pdf>

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