

4-N-hexyl-2-methyl-delta2-thiazoline

Other names:	4-N-hexyl-2-methyl-delta
Inchi:	InChI=1S/C10H19NS/c1-3-4-5-6-7-10-8-12-9(2)11-10/h10H,3-8H2,1-2H3
InchiKey:	QKUVBMICNCFOBQ-UHFFFAOYSA-N
Formula:	C10H19NS
SMILES:	CCCCCCC1CSC(C)=N1
Mol. weight [g/mol]:	185.34

Physical Properties

Property code	Value	Unit	Source
hfus	25.22	kJ/mol	Joback Method
logp	3.491		Crippen Method
mcpvol	162.930	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.26	J/mol×K	549.15	Joback Method
cpg	419.51	J/mol×K	584.94	Joback Method
cpg	436.78	J/mol×K	620.73	Joback Method
cpg	453.10	J/mol×K	656.51	Joback Method
cpg	468.48	J/mol×K	692.30	Joback Method
cpg	482.95	J/mol×K	728.09	Joback Method
cpg	496.52	J/mol×K	763.88	Joback Method

Sources

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=C4145953&Units=SI

Joback Method:

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

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

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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