

DI-4-(2-hydroxyethyl)-2-phenyl-delta2-thiazoline

Other names:	DI-4-(2-hydroxyethyl)-2-phenyl-delta
Inchi:	InChI=1S/C11H13NOS/c13-7-6-10-8-14-11(12-10)9-4-2-1-3-5-9/h1-5,10,13H,6-8H2
InchiKey:	UBOKZTONJAYRSK-UHFFFAOYSA-N
Formula:	C11H13NOS
SMILES:	OCCCC1CSC(c2ccccc2)=N1
Mol. weight [g/mol]:	207.30

Physical Properties

Property code	Value	Unit	Source
hfus	25.94	kJ/mol	Joback Method
logp	1.931		Crippen Method
mcpvol	159.130	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.15	J/mol×K	690.89	Joback Method
cpg	447.38	J/mol×K	730.35	Joback Method
cpg	460.49	J/mol×K	769.81	Joback Method
cpg	472.52	J/mol×K	809.27	Joback Method
cpg	483.52	J/mol×K	848.74	Joback Method
cpg	493.53	J/mol×K	888.20	Joback Method
cpg	502.59	J/mol×K	927.66	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C91132488&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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