Dl-4-(2-hydroxyethyl)-2-phenyl-delta^2-thiazoline

Other names: Dl-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: OCCC1CSC(c2ccccc2)=N1
Mol. weight [g/mol]: 207.29
CAS: 91132-48-8

Physical Properties

Property code	Value	Unit	Source
gf	230.85	kJ/mol	Joback Method
hf	36.95	kJ/mol	Joback Method
hfus	25.94	kJ/mol	Joback Method
hvap	72.27	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	1.931		Crippen Method
mcvol	159.130	ml/mol	McGowan Method
pc	3650.93	kPa	Joback Method
tb	690.89	K	Joback Method
tc	927.66	K	Joback Method
tf	480.14	K	Joback Method
vc	0.585	m3/kmol	Joback 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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91132488&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume