4-Hydroxy-5,5-dimethyl-4-phenylthiazolidine-2-thi

Inchi: InChI=1S/C11H13NOS2/c1-10(2)11(13,12-9(14)15-10)8-6-4-3-5-7-8/h3-7,13H,1-2H3,(H,
InchiKey: MTXXXQTTXHIPDK-UHFFFAOYSA-N
Formula: C11H13NOS2
SMILES: CC1(C)SC(S)=NC1(O)c1ccccc1
Mol. weight [g/mol]: 239.36
CAS: 58417-88-2

Physical Properties

Property code	Value	Unit	Source
gf	241.55	kJ/mol	Joback Method
hf	85.57	kJ/mol	Joback Method
hfus	18.46	kJ/mol	Joback Method
hvap	76.39	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	2.643		Crippen Method
mcvol	175.480	ml/mol	McGowan Method
pc	4249.61	kPa	Joback Method
tb	749.56	K	Joback Method
tc	1021.95	K	Joback Method
tf	560.16	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.52	J/mol×K	749.56	Joback Method
cpg	489.65	J/mol×K	794.96	Joback Method
cpg	504.78	J/mol×K	840.36	Joback Method
cpg	520.28	J/mol×K	885.76	Joback Method
cpg	536.56	J/mol×K	931.16	Joback Method
cpg	554.00	J/mol×K	976.55	Joback Method
cpg	572.99	J/mol×K	1021.95	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=C58417882&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

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