1,5-Benzothiazepin-4(5H)-one, 2-methyl-

Other names: 2-Methyl-1,5-benzothiazepin-4(5H)-one
Inchi: InChI=1S/C10H9NOS/c1-7-6-10(12)11-8-4-2-3-5-9(8)13-7/h2-6H,1H3,(H,11,12)
InchiKey: XMCREDZXYDRQBF-UHFFFAOYSA-N
Formula: C10H9NOS
SMILES: CC1=CC(O)=Nc2ccccc2S1
Mol. weight [g/mol]: 191.25
CAS: 63870-02-0

Physical Properties

Property code	Value	Unit	Source
gf	240.84	kJ/mol	Joback Method
hf	112.77	kJ/mol	Joback Method
hfus	22.72	kJ/mol	Joback Method
hvap	71.97	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	3.284		Crippen Method
mcvol	140.740	ml/mol	McGowan Method
pc	4328.25	kPa	Joback Method
tb	681.80	K	Joback Method
tc	927.39	K	Joback Method
tf	498.91	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.54	J/mol×K	681.80	Joback Method
cpg	365.20	J/mol×K	722.73	Joback Method
cpg	375.91	J/mol×K	763.66	Joback Method
cpg	385.72	J/mol×K	804.59	Joback Method
cpg	394.67	J/mol×K	845.53	Joback Method
cpg	402.78	J/mol×K	886.46	Joback Method
cpg	410.11	J/mol×K	927.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63870020&Units=SI
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

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