

2H-Thiopyran, 3,4-dihydro-

Other names:	Dihydrothiapyran 2,3-Dihydro-4H-thiopyran Thiacyclohex-2-ene
Inchi:	InChI=1S/C5H8S/c1-2-4-6-5-3-1/h2,4H,1,3,5H2
InchiKey:	ATVJJNGVPSKBGO-UHFFFAOYSA-N
Formula:	C5H8S
SMILES:	C1=CSCCC1
Mol. weight [g/mol]:	100.18
CAS:	13042-80-3

Physical Properties

Property code	Value	Unit	Source
gf	93.20	kJ/mol	Joback Method
hf	31.17	kJ/mol	Joback Method
hfus	4.35	kJ/mol	Joback Method
hvap	33.57	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	2.027		Crippen Method
mcvol	82.500	ml/mol	McGowan Method
pc	4890.21	kPa	Joback Method
tb	385.01	K	Joback Method
tc	612.80	K	Joback Method
tf	241.94	K	Joback Method
vc	0.281	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	129.70	J/molxK	385.01	Joback Method
cpg	141.80	J/molxK	422.98	Joback Method
cpg	153.14	J/molxK	460.94	Joback Method
cpg	163.75	J/molxK	498.91	Joback Method
cpg	173.66	J/molxK	536.87	Joback Method
cpg	182.91	J/molxK	574.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13042803&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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