2H-Thiopyran-3(4H)-one, dihydro-

Other names: Dihydro-2H-thiopyran-3(4H)-one
Tetrahydrothiopyran-3-one
1-Thiacyclohexan-3-one
3-Oxotetrahydrothiopyran
3-Thiacyclohexanone
5,6-Dihydro-2(H)-thiopyran-3(4H)-one
Tetrahydrothia-3-pyranone
Inchi: InChI=1S/C5H8OS/c6-5-2-1-3-7-4-5/h1-4H2
InchiKey: ATAMXDLUUTYFKT-UHFFFAOYSA-N
Formula: C5H8OS
SMILES: O=C1CCCSC1
Mol. weight [g/mol]: 116.18
CAS: 19090-03-0

Physical Properties

Property code	Value	Unit	Source
chl	-3531.00 ± 2.50	kJ/mol	NIST Webbook
gf	-59.35	kJ/mol	Joback Method
hf	-133.00 ± 2.60	kJ/mol	NIST Webbook
hfus	2.64	kJ/mol	Joback Method
hvap	49.30 ± 0.10	kJ/mol	NIST Webbook
log10ws	-0.97		Crippen Method
logp	1.083		Crippen Method
mcvol	88.370	ml/mol	McGowan Method
pc	4883.38	kPa	Joback Method
ripol	1541.00		NIST Webbook
tb	453.67	K	Joback Method
tc	701.30	K	Joback Method
tf	309.40	K	Joback Method
vc	0.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	165.39	J/mol×K	453.67	Joback Method
cpg	178.19	J/mol×K	494.94	Joback Method
cpg	190.36	J/mol×K	536.21	Joback Method
cpg	201.88	J/mol×K	577.49	Joback Method
cpg	212.76	J/mol×K	618.76	Joback Method
cpg	222.98	J/mol×K	660.03	Joback Method
cpg	232.53	J/mol×K	701.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19090030&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

chl:	Standard liquid enthalpy of combustion
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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