

Tetrahydro-1,3-oxazine-2-thione

Other names:	Tetrahydro-2H-1,3-oxazine-2-thione
Inchi:	InChI=1S/C4H7NOS/c7-4-5-2-1-3-6-4/h1-3H2,(H,5,7)
InchiKey:	OCWDJXKSTXCEOU-UHFFFAOYSA-N
Formula:	C4H7NOS
SMILES:	SC1=NCCCO1
Mol. weight [g/mol]:	117.17
CAS:	17374-18-4

Physical Properties

Property code	Value	Unit	Source
gf	95.34	kJ/mol	Joback Method
hf	-27.47	kJ/mol	Joback Method
hfus	14.87	kJ/mol	Joback Method
hvap	43.65	kJ/mol	Joback Method
log10ws	-0.71		Crippen Method
logp	0.693		Crippen Method
mcvol	84.260	ml/mol	McGowan Method
pc	6037.30	kPa	Joback Method
rinpol	1115.00		NIST Webbook
tb	462.79	K	Joback Method
tc	719.64	K	Joback Method
tf	400.20	K	Knowledge of a Molecule: An Experimental and Theoretical Study of the Structure and Enthalpy of Formation of Tetrahydro-2H-1,3-oxazine-2-thione
vc	0.303	m3/kmol	

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.20	J/mol×K	462.79	Joback Method
cpg	180.59	J/mol×K	505.60	Joback Method
cpg	192.24	J/mol×K	548.41	Joback Method

cpg	203.16	J/mol×K	591.22	Joback Method
cpg	213.33	J/mol×K	634.02	Joback Method
cpg	222.76	J/mol×K	676.83	Joback Method
cpg	231.43	J/mol×K	719.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17374184&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Knowledge of a Molecule: An Experimental and Theoretical Study of the Structure and Enthalpy of Formation of Tetrahydro-2H-1,3-oxazine-2-thione:	https://www.doi.org/10.1021/je200549z
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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