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

Other names:	Thiopyran-3(2H)-one
Inchi:	InChI=1S/C5H6OS/c6-5-2-1-3-7-4-5/h1,3H,2,4H2
InchiKey:	AEDFDYYPESUHNU-UHFFFAOYSA-N
Formula:	C5H6OS
SMILES:	O=C1CC=CSC1
Mol. weight [g/mol]:	114.17
CAS:	29431-28-5

Physical Properties

Property code	Value	Unit	Source
gf	-29.39	kJ/mol	Joback Method
hf	-106.53	kJ/mol	Joback Method
hfus	3.86	kJ/mol	Joback Method
hvap	37.81	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.206		Crippen Method
mcvol	84.070	ml/mol	McGowan Method
pc	5138.68	kPa	Joback Method
rinpol	1003.00		NIST Webbook
rinpol	1003.00		NIST Webbook
tb	452.83	K	Joback Method
tc	703.24	K	Joback Method
tf	310.16	K	Joback Method
vc	0.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	150.54	J/mol×K	452.83	Joback Method
cpg	161.78	J/mol×K	494.57	Joback Method
cpg	172.44	J/mol×K	536.30	Joback Method
cpg	182.51	J/mol×K	578.04	Joback Method
cpg	191.98	J/mol×K	619.77	Joback Method
cpg	200.85	J/mol×K	661.51	Joback Method

cpg	209.12	J/mol×K	703.24	Joback Method

Sources

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=C29431285&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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