2-Methyl-3,4-dihydro-2H-thiopyran

Inchi: InChI=1S/C6H8OS/c1-5-4-6(7)2-3-8-5/h2-3,5H,4H2,1H3
InchiKey: KGDMIAZBLYJSSW-UHFFFAOYSA-N
Formula: C6H8OS
SMILES: CC1CC(=O)C=CS1
Mol. weight [g/mol]: 128.19

Physical Properties

Property code	Value	Unit	Source
gf	-28.68	kJ/mol	Joback Method
hf	-147.51	kJ/mol	Joback Method
hfus	7.52	kJ/mol	Joback Method
hvap	39.73	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.595		Crippen Method
mcvol	98.160	ml/mol	McGowan Method
pc	4305.56	kPa	Joback Method
rinpol	892.00		NIST Webbook
rinpol	892.00		NIST Webbook
tb	471.04	K	Joback Method
tc	716.73	K	Joback Method
tf	317.19	K	Joback Method
vc	0.344	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.34	J/mol×K	471.04	Joback Method
cpg	204.49	J/mol×K	511.99	Joback Method
cpg	216.99	J/mol×K	552.94	Joback Method
cpg	228.83	J/mol×K	593.89	Joback Method
cpg	240.01	J/mol×K	634.83	Joback Method
cpg	250.51	J/mol×K	675.78	Joback Method
cpg	260.31	J/mol×K	716.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R612203&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume