6-methyltetrahydro-2H-thiopyran-2-one

Inchi: InChI=1S/C6H10OS/c1-5-3-2-4-6(7)8-5/h5H,2-4H2,1H3
InchiKey: DTKFCHDDHQHPAK-UHFFFAOYSA-N
Formula: C6H10OS
SMILES: CC1CCCC(=O)S1
Mol. weight [g/mol]: 130.21

Physical Properties

Property code	Value	Unit	Source
gf	-58.64	kJ/mol	Joback Method
hf	-205.29	kJ/mol	Joback Method
hfus	6.30	kJ/mol	Joback Method
hvap	39.44	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	1.819		Crippen Method
mcvol	102.460	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
rinpol	1124.00		NIST Webbook
rinpol	1124.00		NIST Webbook
ripol	1791.00		NIST Webbook
ripol	1791.00		NIST Webbook
tb	471.88	K	Joback Method
tc	714.89	K	Joback Method
tf	316.43	K	Joback Method
vc	0.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.99	J/mol×K	471.88	Joback Method
cpg	221.62	J/mol×K	512.38	Joback Method
cpg	235.56	J/mol×K	552.88	Joback Method
cpg	248.79	J/mol×K	593.39	Joback Method
cpg	261.30	J/mol×K	633.89	Joback Method
cpg	273.07	J/mol×K	674.39	Joback Method

cpg	284.10	J/mol×K	714.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R301463&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume