2-(mercaptomethyl)thiane

Inchi: InChI=1S/C6H12S2/c7-5-6-3-1-2-4-8-6/h6-7H,1-5H2
InchiKey: YYHUXIOKMLYXRL-UHFFFAOYSA-N
Formula: C6H12S2
SMILES: SCC1CCCCS1
Mol. weight [g/mol]: 148.29

Physical Properties

Property code	Value	Unit	Source
gf	93.34	kJ/mol	Joback Method
hf	-29.11	kJ/mol	Joback Method
hfus	10.83	kJ/mol	Joback Method
hvap	41.93	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.202		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	4266.28	kPa	Joback Method
rinpol	1119.00		NIST Webbook
tb	466.92	K	Joback Method
tc	716.52	K	Joback Method
tf	284.67	K	Joback Method
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.93	J/mol×K	466.92	Joback Method
cpg	244.88	J/mol×K	508.52	Joback Method
cpg	259.81	J/mol×K	550.12	Joback Method
cpg	273.74	J/mol×K	591.72	Joback Method
cpg	286.73	J/mol×K	633.32	Joback Method
cpg	298.80	J/mol×K	674.92	Joback Method
cpg	309.99	J/mol×K	716.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R222538&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