4-(hydroxymethyl)-1,2-dithiepane

Inchi: InChI=1S/C6H12OS2/c7-4-6-2-1-3-8-9-5-6/h6-7H,1-5H2
InchiKey: VLPCHLOFJAZBQI-UHFFFAOYSA-N
Formula: C6H12OS2
SMILES: OCC1CCCSSC1
Mol. weight [g/mol]: 164.29

Physical Properties

Property code	Value	Unit	Source
gf	-45.11	kJ/mol	Joback Method
hf	-180.72	kJ/mol	Joback Method
hfus	12.43	kJ/mol	Joback Method
hvap	57.85	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	1.770		Crippen Method
mcvol	123.110	ml/mol	McGowan Method
pc	4540.80	kPa	Joback Method
tb	548.34	K	Joback Method
tc	777.14	K	Joback Method
tf	388.96	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.74	J/mol×K	548.34	Joback Method
cpg	289.26	J/mol×K	586.47	Joback Method
cpg	301.94	J/mol×K	624.61	Joback Method
cpg	313.82	J/mol×K	662.74	Joback Method
cpg	324.90	J/mol×K	700.88	Joback Method
cpg	335.23	J/mol×K	739.01	Joback Method
cpg	344.80	J/mol×K	777.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R222583&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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