[1,4,5]Oxadithiepane

Other names: 1,4,5-Oxadithiapane
Inchi: InChI=1S/C4H8OS2/c1-3-6-7-4-2-5-1/h1-4H2
InchiKey: DFBDMKHCEZTHOH-UHFFFAOYSA-N
Formula: C4H8OS2
SMILES: C1CSSCCO1
Mol. weight [g/mol]: 136.24
CAS: 3886-40-6

Physical Properties

Property code	Value	Unit	Source
gf	-3.54	kJ/mol	Joback Method
hf	-98.87	kJ/mol	Joback Method
hfus	10.07	kJ/mol	Joback Method
hvap	41.54	kJ/mol	Joback Method
log10ws	-1.24		Crippen Method
logp	1.398		Crippen Method
mcvol	94.930	ml/mol	McGowan Method
pc	5406.57	kPa	Joback Method
rinpol	1162.70		NIST Webbook
rinpol	1118.00		NIST Webbook
rinpol	1118.00		NIST Webbook
rinpol	1172.00		NIST Webbook
tb	442.02	K	Joback Method
tc	698.46	K	Joback Method
tf	336.41	K	Joback Method
vc	0.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	170.60	J/mol×K	442.02	Joback Method
cpg	183.35	J/mol×K	484.76	Joback Method
cpg	195.25	J/mol×K	527.50	Joback Method
cpg	206.33	J/mol×K	570.24	Joback Method

cpg	216.63	J/mol×K	612.98	Joback Method
cpg	226.16	J/mol×K	655.72	Joback Method
cpg	234.95	J/mol×K	698.46	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3886406&Units=SI

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