1-Oxa-4,7-dithionane

Inchi: InChI=1S/C6H14OS2/c1-2-8-5-6-9-4-3-7/h7H,2-6H2,1H3
InchiKey: SLLASBJKZVMFNZ-UHFFFAOYSA-N
Formula: C6H14OS2
SMILES: CCSCCSCCO
Mol. weight [g/mol]: 166.31

Physical Properties

Property code	Value	Unit	Source
gf	-70.94	kJ/mol	Joback Method
hf	-235.66	kJ/mol	Joback Method
hfus	23.64	kJ/mol	Joback Method
hvap	59.26	kJ/mol	Joback Method
log10ws	-1.37		Crippen Method
logp	1.465		Crippen Method
mcvol	133.970	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinpol	1358.00		NIST Webbook
rinpol	1409.30		NIST Webbook
tb	566.42	K	Joback Method
tc	764.78	K	Joback Method
tf	287.00	K	Joback Method
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.50	J/mol×K	566.42	Joback Method
cpg	311.98	J/mol×K	599.48	Joback Method
cpg	321.98	J/mol×K	632.54	Joback Method
cpg	331.48	J/mol×K	665.60	Joback Method
cpg	340.49	J/mol×K	698.66	Joback Method
cpg	349.02	J/mol×K	731.72	Joback Method
cpg	357.07	J/mol×K	764.78	Joback Method

Sources

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=R41463&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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