1,4,7-Oxadithionane

Inchi: InChI=1S/C6H12OS2/c1-3-8-5-6-9-4-2-7-1/h1-6H2
InchiKey: QBAJKVKUJJDYBE-UHFFFAOYSA-N
Formula: C6H12OS2
SMILES: C1CSCCSCCO1
Mol. weight [g/mol]: 164.29
CAS: 40474-73-5

Physical Properties

Property code	Value	Unit	Source
gf	-10.90	kJ/mol	Joback Method
hf	-152.47	kJ/mol	Joback Method
hfus	11.05	kJ/mol	Joback Method
hvap	46.34	kJ/mol	Joback Method
log10ws	-1.08		Crippen Method
logp	1.483		Crippen Method
mcvol	123.110	ml/mol	McGowan Method
pc	4432.62	kPa	Joback Method
rinpol	1358.00		NIST Webbook
rinpol	1421.00		NIST Webbook
tb	496.32	K	Joback Method
tc	764.03	K	Joback Method
tf	351.91	K	Joback Method
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.02	J/mol×K	496.32	Joback Method
cpg	268.77	J/mol×K	540.94	Joback Method
cpg	285.35	J/mol×K	585.56	Joback Method
cpg	300.77	J/mol×K	630.18	Joback Method
cpg	315.02	J/mol×K	674.79	Joback Method
cpg	328.13	J/mol×K	719.41	Joback Method
cpg	340.10	J/mol×K	764.03	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=C40474735&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