

Anti-2-cis-4,5-trimethyl-1,3-oxathiolane

Inchi:	InChI=1S/C6H12OS/c1-4-5(2)8-6(3)7-4/h4-6H,1-3H3
InchiKey:	IWKQZSONTQWRJT-UHFFFAOYSA-N
Formula:	C6H12OS
SMILES:	CC1OC(C)C(C)S1
Mol. weight [g/mol]:	132.22
CAS:	63393-28-2

Physical Properties

Property code	Value	Unit	Source
gf	-25.49	kJ/mol	Joback Method
hf	-234.11	kJ/mol	Joback Method
hfus	19.01	kJ/mol	Joback Method
hvap	38.91	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	1.873		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
tb	417.40	K	Joback Method
tc	629.35	K	Joback Method
tf	269.82	K	Joback Method
vc	0.378	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.82	J/mol×K	417.40	Joback Method
cpg	226.19	J/mol×K	452.73	Joback Method
cpg	239.89	J/mol×K	488.05	Joback Method
cpg	252.95	J/mol×K	523.38	Joback Method
cpg	265.36	J/mol×K	558.70	Joback Method
cpg	277.15	J/mol×K	594.03	Joback Method
cpg	288.33	J/mol×K	629.35	Joback Method

Sources

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=C63393282&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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