cis-2-methyl-4- n-propyl-1,3-oxathiane

Other names: cis-2-methyl-4-propyl-1,3-oxathiane
Inchi: InChI=1S/C8H16OS/c1-3-4-8-5-6-9-7(2)10-8/h7-8H,3-6H2,1-2H3/t7-,8+/m0/s1
InchiKey: GKGOLPMYJJXRGD-JGVFFNPUSA-N
Formula: C8H16OS
SMILES: CCCC1CCOC(C)S1
Mol. weight [g/mol]: 160.28
CAS: 59323-76-1

Physical Properties

Property code	Value	Unit	Source
gf	-13.04	kJ/mol	Joback Method
hf	-261.21	kJ/mol	Joback Method
hfus	21.02	kJ/mol	Joback Method
hvap	43.84	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	2.655		Crippen Method
mcvol	134.940	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
ripol	1514.00		NIST Webbook
ripol	1514.00		NIST Webbook
tb	472.10	K	Joback Method
tc	687.27	K	Joback Method
tf	293.08	K	Joback Method
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.64	J/mol×K	472.10	Joback Method
cpg	312.04	J/mol×K	507.96	Joback Method
cpg	328.56	J/mol×K	543.82	Joback Method
cpg	344.21	J/mol×K	579.69	Joback Method
cpg	359.02	J/mol×K	615.55	Joback Method
cpg	373.01	J/mol×K	651.41	Joback Method

cpg	386.19	J/mol×K	687.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59323761&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume