2-Propyl-1,3-oxothiolane

Inchi: InChI=1S/C6H12OS/c1-2-3-6-7-4-5-8-6/h6H,2-5H2,1H3
InchiKey: FXMKUMPUWACOME-UHFFFAOYSA-N
Formula: C6H12OS
SMILES: CCCC1OCCS1
Mol. weight [g/mol]: 132.22

Physical Properties

Property code	Value	Unit	Source
gf	-10.07	kJ/mol	Joback Method
hf	-193.43	kJ/mol	Joback Method
hfus	16.87	kJ/mol	Joback Method
hvap	39.53	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	1.876		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3768.41	kPa	Joback Method
rinpol	1040.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	1046.00		NIST Webbook
rinpol	1024.00		NIST Webbook
rinpol	1005.00		NIST Webbook
rinpol	1019.00		NIST Webbook
tb	426.74	K	Joback Method
tc	639.53	K	Joback Method
tf	278.30	K	Joback Method
vc	0.380	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.61	J/mol×K	426.74	Joback Method

cpg	224.43	J/mol×K	462.21	Joback Method
cpg	237.50	J/mol×K	497.67	Joback Method
cpg	249.85	J/mol×K	533.14	Joback Method
cpg	261.51	J/mol×K	568.60	Joback Method
cpg	272.51	J/mol×K	604.07	Joback Method
cpg	282.86	J/mol×K	639.53	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=R78894&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

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