trans-2-Methyl-5-propylthiolane

Inchi: InChI=1S/C8H16S/c1-3-4-8-6-5-7(2)9-8/h7-8H,3-6H2,1-2H3/t7-,8-/m1/s1
InchiKey: IWKWEUBLOXWCAL-HTQZYQBOSA-N
Formula: C8H16S
SMILES: CCCC1CCC(C)S1
Mol. weight [g/mol]: 144.28

Physical Properties

Property code	Value	Unit	Source
gf	85.18	kJ/mol	Joback Method
hf	-123.05	kJ/mol	Joback Method
hfus	15.14	kJ/mol	Joback Method
hvap	39.16	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	3.071		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
rinpol	1064.00		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1062.00		NIST Webbook
tb	440.88	K	Joback Method
tc	648.58	K	Joback Method
tf	270.03	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.71	J/mol×K	440.88	Joback Method
cpg	280.64	J/mol×K	475.50	Joback Method
cpg	296.72	J/mol×K	510.11	Joback Method
cpg	311.97	J/mol×K	544.73	Joback Method
cpg	326.43	J/mol×K	579.35	Joback Method
cpg	340.12	J/mol×K	613.97	Joback Method

cpg	353.07	J/mol×K	648.58	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=R41918&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