6-propyl-tetrahydropyran-2-thione

Inchi: InChI=1S/C8H14OS/c1-2-4-7-5-3-6-8(10)9-7/h7H,2-6H2,1H3
InchiKey: AWKFNEOVOOFWMP-UHFFFAOYSA-N
Formula: C8H14OS
SMILES: CCCC1CCCC(=S)O1
Mol. weight [g/mol]: 158.26

Physical Properties

Property code	Value	Unit	Source
gf	45.66	kJ/mol	Joback Method
hf	-171.03	kJ/mol	Joback Method
hfus	22.32	kJ/mol	Joback Method
hvap	45.82	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.683		Crippen Method
mcvol	130.640	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
rinpol	1389.00		NIST Webbook
ripol	2172.00		NIST Webbook
tb	501.58	K	Joback Method
tc	724.18	K	Joback Method
tf	277.54	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.65	J/mol×K	501.58	Joback Method
cpg	302.01	J/mol×K	538.68	Joback Method
cpg	316.42	J/mol×K	575.78	Joback Method
cpg	329.93	J/mol×K	612.88	Joback Method
cpg	342.60	J/mol×K	649.98	Joback Method
cpg	354.46	J/mol×K	687.08	Joback Method
cpg	365.55	J/mol×K	724.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R422565&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume