(E)-6-(pent-3-enyl)-tetrahydropyran-2-thione

Inchi: InChI=1S/C10H16OS/c1-2-3-4-6-9-7-5-8-10(12)11-9/h2-3,9H,4-8H2,1H3/b3-2+
InchiKey: LQWZFGDHWUEUTH-NSCUHMNNSA-N
Formula: C10H16OS
SMILES: CC=CCCC1CCCC(=S)O1
Mol. weight [g/mol]: 184.30

Physical Properties

Property code	Value	Unit	Source
gf	142.72	kJ/mol	Joback Method
hf	-95.09	kJ/mol	Joback Method
hfus	27.71	kJ/mol	Joback Method
hvap	50.23	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.239		Crippen Method
mcvol	154.520	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
rinpol	1595.00		NIST Webbook
rinpol	1595.00		NIST Webbook
ripol	2443.00		NIST Webbook
ripol	2443.00		NIST Webbook
tb	551.50	K	Joback Method
tc	776.61	K	Joback Method
tf	295.00	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.27	J/mol×K	551.50	Joback Method
cpg	376.76	J/mol×K	589.02	Joback Method
cpg	392.17	J/mol×K	626.54	Joback Method
cpg	406.56	J/mol×K	664.05	Joback Method
cpg	420.00	J/mol×K	701.57	Joback Method
cpg	432.55	J/mol×K	739.09	Joback Method

cpg	444.29	J/mol×K	776.61	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R422590&Units=SI

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