6-pentyltetrahydro-2H-thiopyran-2-one

Inchi: InChI=1S/C10H18OS/c1-2-3-4-6-9-7-5-8-10(11)12-9/h9H,2-8H2,1H3
InchiKey: PXRUYLRRFJEVKM-UHFFFAOYSA-N
Formula: C10H18OS
SMILES: CCCCCC1CCCC(=O)S1
Mol. weight [g/mol]: 186.31

Physical Properties

Property code	Value	Unit	Source
gf	-24.96	kJ/mol	Joback Method
hf	-287.85	kJ/mol	Joback Method
hfus	16.66	kJ/mol	Joback Method
hvap	48.34	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.379		Crippen Method
mcvol	158.820	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
rinpol	1565.00		NIST Webbook
ripol	2233.00		NIST Webbook
tb	563.40	K	Joback Method
tc	788.84	K	Joback Method
tf	361.51	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.96	J/mol×K	563.40	Joback Method
cpg	407.66	J/mol×K	600.97	Joback Method
cpg	425.37	J/mol×K	638.55	Joback Method
cpg	442.09	J/mol×K	676.12	Joback Method
cpg	457.82	J/mol×K	713.69	Joback Method
cpg	472.57	J/mol×K	751.27	Joback Method
cpg	486.35	J/mol×K	788.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R301478&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