2-Pentylthiolane

Inchi: InChI=1S/C9H18S/c1-2-3-4-6-9-7-5-8-10-9/h9H,2-8H2,1H3
InchiKey: QQVRCOSRKOIMKB-UHFFFAOYSA-N
Formula: C9H18S
SMILES: CCCCCC1CCCS1
Mol. weight [g/mol]: 158.30

Physical Properties

Property code	Value	Unit	Source
gf	101.31	kJ/mol	Joback Method
hf	-123.35	kJ/mol	Joback Method
hfus	16.66	kJ/mol	Joback Method
hvap	41.70	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.462		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
rinpol	1238.00		NIST Webbook
rinpol	1238.00		NIST Webbook
tb	468.43	K	Joback Method
tc	673.79	K	Joback Method
tf	285.54	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.34	J/mol×K	468.43	Joback Method
cpg	324.89	J/mol×K	502.66	Joback Method
cpg	341.51	J/mol×K	536.88	Joback Method
cpg	357.25	J/mol×K	571.11	Joback Method
cpg	372.13	J/mol×K	605.34	Joback Method
cpg	386.19	J/mol×K	639.56	Joback Method
cpg	399.47	J/mol×K	673.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R583685&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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