2-Butyl-5-methylthiolane

Inchi: InChI=1S/C9H18S/c1-3-4-5-9-7-6-8(2)10-9/h8-9H,3-7H2,1-2H3
InchiKey: FNILMZRAWFXDDT-UHFFFAOYSA-N
Formula: C9H18S
SMILES: CCCCC1CCC(C)S1
Mol. weight [g/mol]: 158.30

Physical Properties

Property code	Value	Unit	Source
gf	93.60	kJ/mol	Joback Method
hf	-143.69	kJ/mol	Joback Method
hfus	17.73	kJ/mol	Joback Method
hvap	41.39	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.461		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
rinpol	1164.00		NIST Webbook
rinpol	1166.00		NIST Webbook
tb	463.76	K	Joback Method
tc	668.83	K	Joback Method
tf	281.30	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.63	J/mol×K	463.76	Joback Method
cpg	325.53	J/mol×K	497.94	Joback Method
cpg	342.54	J/mol×K	532.12	Joback Method
cpg	358.68	J/mol×K	566.29	Joback Method
cpg	373.97	J/mol×K	600.47	Joback Method
cpg	388.46	J/mol×K	634.65	Joback Method
cpg	402.16	J/mol×K	668.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R583581&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume