Thiolane, 2-butyl-5-methyl

Inchi: InChI=1S/C10H20S/c1-3-5-6-10-8-7-9(4-2)11-10/h9-10H,3-8H2,1-2H3
InchiKey: WWHBLJZJOXQRRZ-UHFFFAOYSA-N
Formula: C10H20S
SMILES: CCCCC1CCC(CC)S1
Mol. weight [g/mol]: 172.33

Physical Properties

Property code	Value	Unit	Source
gf	102.02	kJ/mol	Joback Method
hf	-164.33	kJ/mol	Joback Method
hfus	20.32	kJ/mol	Joback Method
hvap	43.61	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.851		Crippen Method
mcvol	157.250	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
rinpol	1164.00		NIST Webbook
tb	486.64	K	Joback Method
tc	688.98	K	Joback Method
tf	292.57	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.53	J/mol×K	486.64	Joback Method
cpg	372.26	J/mol×K	520.36	Joback Method
cpg	390.06	J/mol×K	554.09	Joback Method
cpg	406.96	J/mol×K	587.81	Joback Method
cpg	422.98	J/mol×K	621.54	Joback Method
cpg	438.15	J/mol×K	655.26	Joback Method
cpg	452.50	J/mol×K	688.98	Joback Method

Sources

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=R41598&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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