Naphtho[1,2-b]thiophene, 4-methyl

Inchi: InChI=1S/C13H20S/c1-9-8-10-4-2-3-5-12(10)13-11(9)6-7-14-13/h6-7,9-13H,2-5,8H2,1H3
InchiKey: BSWUMNNOPXJXBY-UHFFFAOYSA-N
Formula: C13H20S
SMILES: CC1CC2CCCCC2C2SC=CC12
Mol. weight [g/mol]: 208.36

Physical Properties

Property code	Value	Unit	Source
gf	246.83	kJ/mol	Joback Method
hf	-55.53	kJ/mol	Joback Method
hfus	22.45	kJ/mol	Joback Method
hvap	50.44	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.078		Crippen Method
mcvol	173.500	ml/mol	McGowan Method
pc	2470.27	kPa	Joback Method
rinpol	314.82		NIST Webbook
rinpol	317.19		NIST Webbook
tb	571.79	K	Joback Method
tc	814.73	K	Joback Method
tf	351.74	K	Joback Method
vc	0.632	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.08	J/mol×K	571.79	Joback Method
cpg	484.53	J/mol×K	612.28	Joback Method
cpg	507.20	J/mol×K	652.77	Joback Method
cpg	528.20	J/mol×K	693.26	Joback Method
cpg	547.65	J/mol×K	733.75	Joback Method
cpg	565.66	J/mol×K	774.24	Joback Method
cpg	582.33	J/mol×K	814.73	Joback Method

Sources

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=R21550&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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