2,4-Dibutyl-2,5-dihydro-thiophene

Inchi: InChI=1S/C12H22S/c1-3-5-7-11-9-12(13-10-11)8-6-4-2/h9,12H,3-8,10H2,1-2H3
InchiKey: XLEWMXIITDXLON-UHFFFAOYSA-N
Formula: C12H22S
SMILES: CCCCC1=CC(CCCC)SC1
Mol. weight [g/mol]: 198.37

Physical Properties

Property code	Value	Unit	Source
gf	146.90	kJ/mol	Joback Method
hf	-138.96	kJ/mol	Joback Method
hfus	25.26	kJ/mol	Joback Method
hvap	49.33	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.409		Crippen Method
mcvol	181.130	ml/mol	McGowan Method
pc	2113.89	kPa	Joback Method
ripol	1573.00		NIST Webbook
tb	541.21	K	Joback Method
tc	741.19	K	Joback Method
tf	332.63	K	Joback Method
vc	0.680	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.59	J/mol×K	541.21	Joback Method
cpg	450.83	J/mol×K	574.54	Joback Method
cpg	468.13	J/mol×K	607.87	Joback Method
cpg	484.54	J/mol×K	641.20	Joback Method
cpg	500.08	J/mol×K	674.53	Joback Method
cpg	514.80	J/mol×K	707.86	Joback Method
cpg	528.71	J/mol×K	741.19	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R495093&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume