2,4-Diethyl-2,5-dihydro-thiophene, stereoisomer 1

Inchi: InChI=1S/C8H14S/c1-3-7-5-8(4-2)9-6-7/h5,8H,3-4,6H2,1-2H3
InchiKey: BZXQFAQLKRFMOG-UHFFFAOYSA-N
Formula: C8H14S
SMILES: CCC1=CC(CC)SC1
Mol. weight [g/mol]: 142.26

Physical Properties

Property code	Value	Unit	Source
gf	113.22	kJ/mol	Joback Method
hf	-56.40	kJ/mol	Joback Method
hfus	14.90	kJ/mol	Joback Method
hvap	40.42	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.848		Crippen Method
mcvol	124.770	ml/mol	McGowan Method
pc	3117.52	kPa	Joback Method
ripol	1377.00		NIST Webbook
ripol	1404.00		NIST Webbook
ripol	1377.00		NIST Webbook
tb	449.69	K	Joback Method
tc	661.33	K	Joback Method
tf	287.55	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.83	J/mol×K	449.69	Joback Method
cpg	264.68	J/mol×K	484.96	Joback Method
cpg	278.75	J/mol×K	520.24	Joback Method
cpg	292.06	J/mol×K	555.51	Joback Method
cpg	304.65	J/mol×K	590.78	Joback Method
cpg	316.54	J/mol×K	626.06	Joback Method
cpg	327.76	J/mol×K	661.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R495102&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume