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

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]: 142.27

Physical Properties

Property code	Value	Unit	Source
hfus	14.90	kJ/mol	Joback Method
logp	2.848		Crippen Method
mcvol	124.770	ml/mol	McGowan Method
ripol	1377.00		NIST Webbook
ripol	1404.00		NIST Webbook
ripol	1377.00		NIST Webbook

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R495102&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices