2-Ethyl-4,5-dihydrothiophene

Other names: 4,5-dihydro-2-ethylthiophene
Inchi: InChI=1S/C6H10S/c1-2-6-4-3-5-7-6/h4H,2-3,5H2,1H3
InchiKey: VBOZZIMZLMYLBC-UHFFFAOYSA-N
Formula: C6H10S
SMILES: CCC1=CCCS1
Mol. weight [g/mol]: 114.21

Physical Properties

Property code	Value	Unit	Source
gf	104.09	kJ/mol	Joback Method
hf	5.22	kJ/mol	Joback Method
hfus	8.65	kJ/mol	Joback Method
hvap	36.28	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.417		Crippen Method
mcvol	96.590	ml/mol	McGowan Method
pc	4077.71	kPa	Joback Method
ripol	1362.00		NIST Webbook
ripol	1368.00		NIST Webbook
ripol	1362.00		NIST Webbook
tb	408.60	K	Joback Method
tc	626.01	K	Joback Method
tf	269.25	K	Joback Method
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.78	J/mol×K	408.60	Joback Method
cpg	181.81	J/mol×K	444.84	Joback Method
cpg	193.14	J/mol×K	481.07	Joback Method
cpg	203.80	J/mol×K	517.31	Joback Method
cpg	213.81	J/mol×K	553.54	Joback Method
cpg	223.22	J/mol×K	589.78	Joback Method

cpg	232.04	J/mol×K	626.01	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=R298976&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