4-Ethylthiane

Other names: 4-Ethyltetrahydro-2H-thiopyran
4-Ethyl-thiacyclohexane
Inchi: InChI=1S/C7H14S/c1-2-7-3-5-8-6-4-7/h7H,2-6H2,1H3
InchiKey: DZXVHXPCUHPSMD-UHFFFAOYSA-N
Formula: C7H14S
SMILES: CCC1CCSCC1
Mol. weight [g/mol]: 130.25
CAS: 40324-31-0

Physical Properties

Property code	Value	Unit	Source
gf	72.37	kJ/mol	Joback Method
hf	-88.23	kJ/mol	Joback Method
hfus	9.38	kJ/mol	Joback Method
hvap	37.42	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.540		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	3497.14	kPa	Joback Method
rinpol	1050.00		NIST Webbook
rinpol	1050.00		NIST Webbook
tb	426.94	K	Joback Method
tc	646.42	K	Joback Method
tf	259.48	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.37	J/mol×K	426.94	Joback Method
cpg	236.92	J/mol×K	463.52	Joback Method
cpg	252.59	J/mol×K	500.10	Joback Method
cpg	267.39	J/mol×K	536.68	Joback Method
cpg	281.37	J/mol×K	573.26	Joback Method

cpg	294.54	J/mol×K	609.84	Joback Method
cpg	306.93	J/mol×K	646.42	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=C40324310&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