

Thiazole, 2-ethyl-4,5-dihydro-

Other names:	2-Ethylthiazoline 2-Ethyl-4,5-dihydro-1,3-thiazole 2-Ethyl-2-thiazoline 2-Ethyl-4,5-dihydrothiazole
Inchi:	InChI=1S/C5H9NS/c1-2-5-6-3-4-7-5/h2-4H2,1H3
InchiKey:	VBLYWGDAYORRDM-UHFFFAOYSA-N
Formula:	C5H9NS
SMILES:	CCC1=NCCS1
Mol. weight [g/mol]:	115.20
CAS:	16982-46-0

Physical Properties

Property code	Value	Unit	Source
gf	212.45	kJ/mol	Joback Method
hf	96.83	kJ/mol	Joback Method
hfus	11.20	kJ/mol	Joback Method
hvap	40.27	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	1.542		Crippen Method
mcvol	92.480	ml/mol	McGowan Method
pc	4634.00	kPa	Joback Method
rinpol	924.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	958.00		NIST Webbook
ripol	1364.00		NIST Webbook
ripol	1364.00		NIST Webbook
ripol	1368.00		NIST Webbook
ripol	1368.00		NIST Webbook
tb	439.42	K	Joback Method
tc	672.98	K	Joback Method
tf	329.52	K	Joback Method
vc	0.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.70	J/mol×K	439.42	Joback Method
cpg	192.40	J/mol×K	478.35	Joback Method
cpg	204.39	J/mol×K	517.27	Joback Method
cpg	215.70	J/mol×K	556.20	Joback Method
cpg	226.32	J/mol×K	595.13	Joback Method
cpg	236.29	J/mol×K	634.06	Joback Method
cpg	245.61	J/mol×K	672.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16982460&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	http://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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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