2-Butylthiazoline

Other names: 2-Butyl-4,5-dihydro-1,3-thiazole
Thiazole, 2-butyl-4,5-dihydro
4,5-Dihydro-2-butylthiazole
Inchi: InChI=1S/C7H13NS/c1-2-3-4-7-8-5-6-9-7/h2-6H2,1H3
InchiKey: NTJAWQUVLBPTQF-UHFFFAOYSA-N
Formula: C7H13NS
SMILES: CCCCC1=NCCS1
Mol. weight [g/mol]: 143.25
CAS: 28221-34-3

Physical Properties

Property code	Value	Unit	Source
gf	229.29	kJ/mol	Joback Method
hf	55.55	kJ/mol	Joback Method
hfus	16.38	kJ/mol	Joback Method
hvap	44.72	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	2.322		Crippen Method
mcvol	120.660	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
rinpol	1123.00		NIST Webbook
tb	485.18	K	Joback Method
tc	711.29	K	Joback Method
tf	352.06	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.03	J/mol×K	485.18	Joback Method
cpg	277.24	J/mol×K	522.86	Joback Method
cpg	291.61	J/mol×K	560.55	Joback Method
cpg	305.14	J/mol×K	598.23	Joback Method
cpg	317.88	J/mol×K	635.92	Joback Method

cpg	329.83	J/mol×K	673.60	Joback Method
cpg	341.01	J/mol×K	711.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28221343&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

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