2-Isopropyl-4,5-dihydrothiazole

Inchi: InChI=1S/C6H11NS/c1-5(2)6-7-3-4-8-6/h5H,3-4H2,1-2H3
InchiKey: HTSOMKXWOBFXMF-UHFFFAOYSA-N
Formula: C6H11NS
SMILES: CC(C)C1=NCCS1
Mol. weight [g/mol]: 129.22

Physical Properties

Property code	Value	Unit	Source
gf	218.43	kJ/mol	Joback Method
hf	70.91	kJ/mol	Joback Method
hfus	10.26	kJ/mol	Joback Method
hvap	42.10	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	1.788		Crippen Method
mcvol	106.570	ml/mol	McGowan Method
pc	4124.99	kPa	Joback Method
ripol	1355.00		NIST Webbook
ripol	1355.00		NIST Webbook
tb	461.86	K	Joback Method
tc	697.46	K	Joback Method
tf	325.79	K	Joback Method
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.97	J/mol×K	461.86	Joback Method
cpg	234.46	J/mol×K	501.13	Joback Method
cpg	248.11	J/mol×K	540.39	Joback Method
cpg	260.95	J/mol×K	579.66	Joback Method
cpg	273.00	J/mol×K	618.93	Joback Method
cpg	284.27	J/mol×K	658.20	Joback Method
cpg	294.79	J/mol×K	697.46	Joback Method

Sources

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=R640852&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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