5,6-Dihydro-2-ethyl-4,6-dimethyl-4H-1,3,5-dithiazi

Other names: 2-Ethyl-4,6-dimethyl-[1,3,5]dithiazinane
1,3,5-Dithiazine, perhydro-2-ethyl-4,6-dimethyl
Inchi: InChI=1S/C7H15NS2/c1-4-7-9-5(2)8-6(3)10-7/h5-8H,4H2,1-3H3
InchiKey: BHTMBVSWSZTUBT-UHFFFAOYSA-N
Formula: C7H15NS2
SMILES: CCC1SC(C)NC(C)S1
Mol. weight [g/mol]: 177.33

Physical Properties

Property code	Value	Unit	Source
gf	184.52	kJ/mol	Joback Method
hf	-45.84	kJ/mol	Joback Method
hfus	24.77	kJ/mol	Joback Method
hvap	49.37	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.484		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
rinpol	1282.00		NIST Webbook
rinpol	1279.00		NIST Webbook
ripol	1750.00		NIST Webbook
ripol	1750.00		NIST Webbook
tb	513.98	K	Joback Method
tc	754.24	K	Joback Method
tf	439.48	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.63	J/mol×K	513.98	Joback Method
cpg	329.14	J/mol×K	554.02	Joback Method
cpg	345.73	J/mol×K	594.07	Joback Method
cpg	361.40	J/mol×K	634.11	Joback Method

cpg	376.16	J/mol×K	674.15	Joback Method
cpg	390.00	J/mol×K	714.20	Joback Method
cpg	402.94	J/mol×K	754.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R62243&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
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