5,6-Dihydro-2,6-diethyl-4-methyl-4H-1,3,5-dithiazi

Other names: 5,6-Dihydro-6-methyl-2,4-diethyl-4H-1,3,5-dithiazine
Inchi: InChI=1S/C8H17NS2/c1-4-7-9-6(3)10-8(5-2)11-7/h6-9H,4-5H2,1-3H3
InchiKey: AQKSWRRFZAIKOU-UHFFFAOYSA-N
Formula: C8H17NS2
SMILES: CCC1NC(C)SC(CC)S1
Mol. weight [g/mol]: 191.36

Physical Properties

Property code	Value	Unit	Source
gf	192.94	kJ/mol	Joback Method
hf	-66.48	kJ/mol	Joback Method
hfus	27.36	kJ/mol	Joback Method
hvap	51.59	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	2.874		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
rinpol	1348.40		NIST Webbook
rinpol	1348.40		NIST Webbook
tb	536.86	K	Joback Method
tc	772.45	K	Joback Method
tf	450.75	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.00	J/mol×K	536.86	Joback Method
cpg	376.45	J/mol×K	576.13	Joback Method
cpg	393.91	J/mol×K	615.39	Joback Method
cpg	410.39	J/mol×K	654.66	Joback Method
cpg	425.90	J/mol×K	693.92	Joback Method
cpg	440.44	J/mol×K	733.19	Joback Method
cpg	454.03	J/mol×K	772.45	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=R253220&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume