1,3,5-Dithiazine, perhydro-4-methyl-2,6-bis-(1-methylethyl)

Other names: 5,6-Dihydro-4-methyl-2,6-diisopropyl-4H-1,3,5-dithiazine
Inchi: InChI=1S/C10H21NS2/c1-6(2)9-11-8(5)12-10(13-9)7(3)4/h6-11H,1-5H3
InchiKey: VDCMBNABIUZUMB-UHFFFAOYSA-N
Formula: C10H21NS2
SMILES: CC1NC(C(C)C)SC(C(C)C)S1
Mol. weight [g/mol]: 219.41

Physical Properties

Property code	Value	Unit	Source
gf	204.90	kJ/mol	Joback Method
hf	-118.32	kJ/mol	Joback Method
hfus	25.49	kJ/mol	Joback Method
hvap	55.27	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.366		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	2475.19	kPa	Joback Method
rinpol	1492.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1490.00		NIST Webbook
tb	581.74	K	Joback Method
tc	818.59	K	Joback Method
tf	443.29	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.75	J/mol×K	581.74	Joback Method
cpg	477.63	J/mol×K	621.22	Joback Method
cpg	497.30	J/mol×K	660.69	Joback Method
cpg	515.77	J/mol×K	700.17	Joback Method
cpg	533.05	J/mol×K	739.64	Joback Method
cpg	549.17	J/mol×K	779.12	Joback Method

cpg	564.13	J/mol×K	818.59	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=R62275&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