1,3,5-Dithiazine, perhydro-2,6-dibutyl-4-methyl

Inchi: InChI=1S/C12H25NS2/c1-4-6-8-11-13-10(3)14-12(15-11)9-7-5-2/h10-13H,4-9H2,1-3H3
InchiKey: FUHPSDAXOVSFJY-UHFFFAOYSA-N
Formula: C12H25NS2
SMILES: CCCCC1NC(C)SC(CCCC)S1
Mol. weight [g/mol]: 247.46

Physical Properties

Property code	Value	Unit	Source
gf	226.62	kJ/mol	Joback Method
hf	-149.04	kJ/mol	Joback Method
hfus	37.72	kJ/mol	Joback Method
hvap	60.50	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	4.435		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpol	1641.00		NIST Webbook
rinpol	1641.00		NIST Webbook
tb	628.38	K	Joback Method
tc	846.81	K	Joback Method
tf	495.83	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.51	J/mol×K	628.38	Joback Method
cpg	581.29	J/mol×K	664.78	Joback Method
cpg	600.90	J/mol×K	701.19	Joback Method
cpg	619.38	J/mol×K	737.59	Joback Method
cpg	636.74	J/mol×K	774.00	Joback Method
cpg	653.00	J/mol×K	810.40	Joback Method
cpg	668.18	J/mol×K	846.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R62225&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