5,6-Dihydro-2,4,6-triisopropyl-4H-1,3,5-dithiazine

Other names: 2,4,6-Tri-isopropyl-[1,3,5]dithiazinane
Inchi: InChI=1S/C12H25NS2/c1-7(2)10-13-11(8(3)4)15-12(14-10)9(5)6/h7-13H,1-6H3
InchiKey: NRIFWWMNTMXTRB-UHFFFAOYSA-N
Formula: C12H25NS2
SMILES: CC(C)C1NC(C(C)C)SC(C(C)C)S1
Mol. weight [g/mol]: 247.46

Physical Properties

Property code	Value	Unit	Source
gf	219.30	kJ/mol	Joback Method
hf	-164.88	kJ/mol	Joback Method
hfus	27.15	kJ/mol	Joback Method
hvap	59.33	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.002		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
ripol	1930.00		NIST Webbook
ripol	1930.00		NIST Webbook
tb	627.06	K	Joback Method
tc	859.45	K	Joback Method
tf	450.83	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.68	J/mol×K	627.06	Joback Method
cpg	583.92	J/mol×K	665.79	Joback Method
cpg	604.82	J/mol×K	704.52	Joback Method
cpg	624.39	J/mol×K	743.26	Joback Method
cpg	642.66	J/mol×K	781.99	Joback Method
cpg	659.64	J/mol×K	820.72	Joback Method
cpg	675.38	J/mol×K	859.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R253240&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume