1,3,5-Dithiazine, perhydro-4,6-dimethyl-2-pentyl

Inchi: InChI=1S/C10H21NS2/c1-4-5-6-7-10-12-8(2)11-9(3)13-10/h8-11H,4-7H2,1-3H3
InchiKey: MOQYJFGRWHTLRP-UHFFFAOYSA-N
Formula: C10H21NS2
SMILES: CCCCCC1SC(C)NC(C)S1
Mol. weight [g/mol]: 219.41

Physical Properties

Property code	Value	Unit	Source
gf	209.78	kJ/mol	Joback Method
hf	-107.76	kJ/mol	Joback Method
hfus	32.54	kJ/mol	Joback Method
hvap	56.05	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.654		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
rinpol	1571.00		NIST Webbook
rinpol	1571.00		NIST Webbook
tb	582.62	K	Joback Method
tc	809.24	K	Joback Method
tf	473.29	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.06	J/mol×K	582.62	Joback Method
cpg	475.93	J/mol×K	620.39	Joback Method
cpg	494.70	J/mol×K	658.16	Joback Method
cpg	512.40	J/mol×K	695.93	Joback Method
cpg	529.04	J/mol×K	733.70	Joback Method
cpg	544.63	J/mol×K	771.47	Joback Method
cpg	559.20	J/mol×K	809.24	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R54492&Units=SI

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