1,3,5-Dithiazine, 4-butyl-2-mehyl-6-pentyl

Inchi: InChI=1S/C13H27NS2/c1-4-6-8-10-13-14-12(9-7-5-2)15-11(3)16-13/h11-14H,4-10H2,1-3
InchiKey: YSHOAYUYWBSGHO-UHFFFAOYSA-N
Formula: C13H27NS2
SMILES: CCCCCC1NC(CCCC)SC(C)S1
Mol. weight [g/mol]: 261.49

Physical Properties

Property code	Value	Unit	Source
gf	235.04	kJ/mol	Joback Method
hf	-169.68	kJ/mol	Joback Method
hfus	40.31	kJ/mol	Joback Method
hvap	62.72	kJ/mol	Joback Method
log10ws	-5.94		Crippen Method
logp	4.825		Crippen Method
mcvol	225.850	ml/mol	McGowan Method
pc	1867.55	kPa	Joback Method
rinpol	1849.00		NIST Webbook
rinpol	1849.00		NIST Webbook
tb	651.26	K	Joback Method
tc	866.00	K	Joback Method
tf	507.10	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.88	J/mol×K	651.26	Joback Method
cpg	635.96	J/mol×K	687.05	Joback Method
cpg	655.86	J/mol×K	722.84	Joback Method
cpg	674.59	J/mol×K	758.63	Joback Method
cpg	692.19	J/mol×K	794.42	Joback Method
cpg	708.67	J/mol×K	830.21	Joback Method
cpg	724.05	J/mol×K	866.00	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=R54474&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