1,2,4,5-Tetrazine, 1,4-dihydro-3,6-dimethyl-

Other names: 1,2,4,5-Tetrazine, 3,6-dihydro-3,6-dimethyl-
Inchi: InChI=1S/C4H8N4/c1-3-5-7-4(2)8-6-3/h1-2H3,(H,5,6)(H,7,8)
InchiKey: DPHZUYOKHNJDLR-UHFFFAOYSA-N
Formula: C4H8N4
SMILES: CC1=NN=C(C)NN1
Mol. weight [g/mol]: 112.13
CAS: 37454-64-1

Physical Properties

Property code	Value	Unit	Source
gf	464.60	kJ/mol	Joback Method
hf	258.95	kJ/mol	Joback Method
hfus	28.00	kJ/mol	Joback Method
hvap	53.08	kJ/mol	Joback Method
ie	7.85	eV	NIST Webbook
log10ws	-1.07		Crippen Method
logp	-0.154		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
pc	6200.01	kPa	Joback Method
tb	527.92	K	Joback Method
tc	787.53	K	Joback Method
tf	526.16	K	Joback Method
vc	0.338	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.23	J/mol×K	527.92	Joback Method
cpg	218.74	J/mol×K	571.19	Joback Method
cpg	231.62	J/mol×K	614.46	Joback Method
cpg	243.82	J/mol×K	657.73	Joback Method
cpg	255.25	J/mol×K	700.99	Joback Method
cpg	265.84	J/mol×K	744.26	Joback Method
cpg	275.50	J/mol×K	787.53	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=C37454641&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume