3-Phenyl-2-piperazinene

Inchi: InChI=1S/C10H12N2O/c13-10-9(11-6-7-12-10)8-4-2-1-3-5-8/h1-5,9,11H,6-7H2,(H,12,13)
InchiKey: WKFFHKBGGZHQAX-UHFFFAOYSA-N
Formula: C10H12N2O
SMILES: O=C1NCCNC1c1ccccc1
Mol. weight [g/mol]: 176.22
CAS: 5368-28-5

Physical Properties

Property code	Value	Unit	Source
gf	223.01	kJ/mol	Joback Method
hf	-20.96	kJ/mol	Joback Method
hfus	26.22	kJ/mol	Joback Method
hvap	58.32	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	0.447		Crippen Method
mcvol	138.670	ml/mol	McGowan Method
pc	4124.99	kPa	Joback Method
tb	639.35	K	Joback Method
tc	912.32	K	Joback Method
tf	514.54	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.65	J/mol×K	639.35	Joback Method
cpg	376.89	J/mol×K	684.84	Joback Method
cpg	393.71	J/mol×K	730.34	Joback Method
cpg	409.10	J/mol×K	775.83	Joback Method
cpg	423.04	J/mol×K	821.33	Joback Method
cpg	435.51	J/mol×K	866.82	Joback Method
cpg	446.49	J/mol×K	912.32	Joback Method

Sources

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=C5368285&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume