Cyclopentylidenephenylacetonitrile

Inchi: InChI=1S/C13H13N/c14-10-13(12-8-4-5-9-12)11-6-2-1-3-7-11/h1-3,6-7H,4-5,8-9H2
InchiKey: OMNFRAFCXNVDLP-UHFFFAOYSA-N
Formula: C13H13N
SMILES: N#CC(=C1CCCC1)c1ccccc1
Mol. weight [g/mol]: 183.25
CAS: 21713-75-7

Physical Properties

Property code	Value	Unit	Source
chs	-7199.00	kJ/mol	NIST Webbook
gf	385.34	kJ/mol	Joback Method
hf	236.82	kJ/mol	Joback Method
hfs	225.40	kJ/mol	NIST Webbook
hfus	16.85	kJ/mol	Joback Method
hvap	58.72	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.538		Crippen Method
mcvol	156.490	ml/mol	McGowan Method
pc	2732.56	kPa	Joback Method
tb	652.07	K	Joback Method
tc	906.02	K	Joback Method
tf	339.22	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.18	J/mol×K	652.07	Joback Method
cpg	409.64	J/mol×K	694.39	Joback Method
cpg	423.83	J/mol×K	736.72	Joback Method
cpg	436.87	J/mol×K	779.04	Joback Method
cpg	448.86	J/mol×K	821.37	Joback Method
cpg	459.91	J/mol×K	863.69	Joback Method
cpg	470.12	J/mol×K	906.02	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=C21713757&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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