Benzeneacetonitrile, «alpha»-cyclohexylidene

Other names: Cyclohexylidenephenylacetonitrile
2-cyclohexyl-2-cyclohexylideneacetonitrile
Inchi: InChI=1S/C14H15N/c15-11-14(12-7-3-1-4-8-12)13-9-5-2-6-10-13/h1,3-4,7-8H,2,5-6,9-10
InchiKey: ZHOOOLQOWQVYOE-UHFFFAOYSA-N
Formula: C14H15N
SMILES: N#CC(=C1CCCCC1)c1ccccc1
Mol. weight [g/mol]: 197.28
CAS: 10461-98-0

Physical Properties

Property code	Value	Unit	Source
chs	-7857.72	kJ/mol	NIST Webbook
gf	381.66	kJ/mol	Joback Method
hf	210.02	kJ/mol	Joback Method
hfs	204.80	kJ/mol	NIST Webbook
hfus	17.34	kJ/mol	Joback Method
hvap	61.12	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.928		Crippen Method
mcvol	170.580	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
tb	679.22	K	Joback Method
tc	935.77	K	Joback Method
tf	346.97	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.89	J/mol×K	679.22	Joback Method
cpg	463.70	J/mol×K	721.98	Joback Method
cpg	479.13	J/mol×K	764.74	Joback Method
cpg	493.27	J/mol×K	807.49	Joback Method
cpg	506.23	J/mol×K	850.25	Joback Method

cpg	518.10	J/mol×K	893.01	Joback Method
cpg	528.99	J/mol×K	935.77	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=C10461980&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