.alpha.-Cyclohexylphenylacetonitrile

Other names: «alpha»-Cyclohexylphenylacetonitrile
Benzeneacetonitrile, «alpha»-cyclohexyl-
Inchi: InChI=1S/C14H17N/c15-11-14(12-7-3-1-4-8-12)13-9-5-2-6-10-13/h1,3-4,7-8,13-14H,2,5-
InchiKey: IZSWBXTYTALSOZ-UHFFFAOYSA-N
Formula: C14H17N
SMILES: N#CC(c1ccccc1)C1CCCCC1
Mol. weight [g/mol]: 199.30

Physical Properties

Property code	Value	Unit	Source
hf	156.55	kJ/mol	Cheméo Relay (1.0)
hfus	15.88	kJ/mol	Joback Method
hvap	76.28	kJ/mol	Cheméo Relay (1.0)
logp	3.874		Crippen Method
mcvol	174.880	ml/mol	McGowan Method
tb	578.27	K	Cheméo Relay (1.0)
tf	326.23	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.87	J/mol×K	667.59	Joback Method
cpg	492.51	J/mol×K	709.29	Joback Method
cpg	509.64	J/mol×K	750.98	Joback Method
cpg	525.36	J/mol×K	792.68	Joback Method
cpg	539.73	J/mol×K	834.38	Joback Method
cpg	552.85	J/mol×K	876.07	Joback Method
cpg	564.78	J/mol×K	917.77	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3893230&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point