4-Benzylphenylacetonitrile

Inchi: InChI=1S/C15H13N/c16-11-10-13-6-8-15(9-7-13)12-14-4-2-1-3-5-14/h1-9H,10,12H2
InchiKey: RNZDBGKQDKFAPR-UHFFFAOYSA-N
Formula: C15H13N
SMILES: N#CCc1ccc(Cc2ccccc2)cc1
Mol. weight [g/mol]: 207.27
CAS: 101096-72-4

Physical Properties

Property code	Value	Unit	Source
gf	423.79	kJ/mol	Joback Method
hf	273.54	kJ/mol	Joback Method
hfus	23.81	kJ/mol	Joback Method
hvap	64.68	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.343		Crippen Method
mcvol	176.070	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
tb	703.02	K	Joback Method
tc	950.93	K	Joback Method
tf	389.16	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.70	J/mol×K	703.02	Joback Method
cpg	463.97	J/mol×K	744.34	Joback Method
cpg	477.08	J/mol×K	785.66	Joback Method
cpg	489.12	J/mol×K	826.97	Joback Method
cpg	500.15	J/mol×K	868.29	Joback Method
cpg	510.27	J/mol×K	909.61	Joback Method
cpg	519.55	J/mol×K	950.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C101096724&Units=SI
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

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