3-Benzyloxyphenylacetonitrile

Other names: Benzeneacetonitrile, 3-(phenylmethoxy)-
Inchi: InChI=1S/C15H13NO/c16-10-9-13-7-4-8-15(11-13)17-12-14-5-2-1-3-6-14/h1-8,11H,9,12
InchiKey: CKZFVIPFANUBDW-UHFFFAOYSA-N
Formula: C15H13NO
SMILES: N#CCc1cccc(OCc2ccccc2)c1
Mol. weight [g/mol]: 223.27
CAS: 20967-96-8

Physical Properties

Property code	Value	Unit	Source
gf	318.79	kJ/mol	Joback Method
hf	141.32	kJ/mol	Joback Method
hfus	24.99	kJ/mol	Joback Method
hvap	67.09	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.332		Crippen Method
mcvol	181.940	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
tb	725.44	K	Joback Method
tc	969.36	K	Joback Method
tf	411.39	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.74	J/mol×K	725.44	Joback Method
cpg	488.60	J/mol×K	766.09	Joback Method
cpg	501.34	J/mol×K	806.75	Joback Method
cpg	513.00	J/mol×K	847.40	Joback Method
cpg	523.64	J/mol×K	888.05	Joback Method
cpg	533.30	J/mol×K	928.70	Joback Method
cpg	542.06	J/mol×K	969.36	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20967968&Units=SI

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