4-Benzyloxy-3-methoxyphenylacetonitrile

Inchi: InChI=1S/C16H15NO2/c1-18-16-11-13(9-10-17)7-8-15(16)19-12-14-5-3-2-4-6-14/h2-8,11
InchiKey: KSOYPRFHKIOHMY-UHFFFAOYSA-N
Formula: C16H15NO2
SMILES: COc1cc(CC#N)ccc1OCc1ccccc1
Mol. weight [g/mol]: 253.30
CAS: 1700-29-4

Physical Properties

Property code	Value	Unit	Source
gf	212.58	kJ/mol	Joback Method
hf	-23.01	kJ/mol	Joback Method
hfus	28.38	kJ/mol	Joback Method
hvap	72.38	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.340		Crippen Method
mcvol	201.900	ml/mol	McGowan Method
pc	2102.27	kPa	Joback Method
tb	775.72	K	Joback Method
tc	1012.21	K	Joback Method
tf	457.41	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.89	J/mol×K	775.72	Joback Method
cpg	565.59	J/mol×K	815.14	Joback Method
cpg	578.16	J/mol×K	854.55	Joback Method
cpg	589.62	J/mol×K	893.97	Joback Method
cpg	599.99	J/mol×K	933.38	Joback Method
cpg	609.31	J/mol×K	972.80	Joback Method
cpg	617.59	J/mol×K	1012.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1700294&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