4-Butoxyphenylacetonitrile

Inchi: InChI=1S/C12H15NO/c1-2-3-10-14-12-6-4-11(5-7-12)8-9-13/h4-7H,2-3,8,10H2,1H3
InchiKey: SKTHXBXIQFAXPC-UHFFFAOYSA-N
Formula: C12H15NO
SMILES: CCCCOc1ccc(CC#N)cc1
Mol. weight [g/mol]: 189.25
CAS: 38746-93-9

Physical Properties

Property code	Value	Unit	Source
gf	181.12	kJ/mol	Joback Method
hf	-33.29	kJ/mol	Joback Method
hfus	23.18	kJ/mol	Joback Method
hvap	58.13	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.932		Crippen Method
mcvol	163.430	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
tb	630.12	K	Joback Method
tc	844.01	K	Joback Method
tf	351.16	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.16	J/mol×K	630.12	Joback Method
cpg	419.77	J/mol×K	665.77	Joback Method
cpg	432.60	J/mol×K	701.42	Joback Method
cpg	444.66	J/mol×K	737.06	Joback Method
cpg	455.98	J/mol×K	772.71	Joback Method
cpg	466.57	J/mol×K	808.36	Joback Method
cpg	476.45	J/mol×K	844.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38746939&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

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