Benzeneacetonitrile, 3,4-diethoxy-

Other names: (3,4-diethoxyphenyl)acetonitrile
Inchi: InChI=1S/C12H15NO2/c1-3-14-11-6-5-10(7-8-13)9-12(11)15-4-2/h5-6,9H,3-4,7H2,1-2H3
InchiKey: OBDKFHFLERWBBI-UHFFFAOYSA-N
Formula: C12H15NO2
SMILES: CCOc1ccc(CC#N)cc1OCC
Mol. weight [g/mol]: 205.25
CAS: 27472-21-5

Physical Properties

Property code	Value	Unit	Source
gf	66.49	kJ/mol	Joback Method
hf	-176.98	kJ/mol	Joback Method
hfus	23.98	kJ/mol	Joback Method
hvap	61.20	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	2.550		Crippen Method
mcvol	169.300	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
tb	657.52	K	Joback Method
tc	869.91	K	Joback Method
tf	385.91	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.14	J/mol×K	657.52	Joback Method
cpg	443.37	J/mol×K	692.92	Joback Method
cpg	455.87	J/mol×K	728.32	Joback Method
cpg	467.64	J/mol×K	763.72	Joback Method
cpg	478.68	J/mol×K	799.11	Joback Method
cpg	488.98	J/mol×K	834.51	Joback Method
cpg	498.54	J/mol×K	869.91	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=C27472215&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