4'-BUTOXY-4-BIPHENYLCARBONITRILE

Other names:	4'-Butoxy-4-biphenylcarbonitrile
	4'-n-Butyloxy-4-cyanobiphenyl
	4-Cyano-4'-n-butoxybiphenyl
	4'-butoxy[1,1'-biphenyl]-4-carbonitrile
Inchi:	InChI=1S/C17H17NO/c1-2-3-12-19-17-10-8-16(9-11-17)15-6-4-14(13-18)5-7-15/h4-11H,
InchiKey:	KPQVQWUNELODQE-UHFFFAOYSA-N
Formula:	C17H17NO
SMILES:	CCCCOc1ccc(-c2ccc(C#N)cc2)cc1
Mol. weight [g/mol]:	251.33

Physical Properties

Property code	Value	Unit	Source
hf	71.40	kJ/mol	Cheméo Relay (1.0)
hfus	29.78	kJ/mol	Joback Method
ie	8.36	eV	Cheméo Relay (1.0)
logp	4.404		Crippen Method
mcvol	210.120	ml/mol	McGowan Method
tb	665.98	K	Cheméo Relay (1.0)
tc	889.41	K	Cheméo Relay (1.0)
tf	351.00 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.98	J/mol×K	776.18	Joback Method
cpg	594.46	J/mol×K	815.41	Joback Method
cpg	607.81	J/mol×K	854.64	Joback Method
cpg	620.08	J/mol×K	893.88	Joback Method
cpg	631.31	J/mol×K	933.11	Joback Method
cpg	641.56	J/mol×K	972.34	Joback Method
cpg	650.88	J/mol×K	1011.57	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52709872&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point