4-Ethoxy-4'-butylazobenzene

Inchi: InChI=1S/C18H22N2O/c1-3-5-6-15-7-9-16(10-8-15)19-20-17-11-13-18(14-12-17)21-4-2/h
InchiKey: VWOMPNGMNROKFP-UHFFFAOYSA-N
Formula: C18H22N2O
SMILES: CCCCc1ccc(N=Nc2ccc(OCC)cc2)cc1
Mol. weight [g/mol]: 282.39

Physical Properties

Property code	Value	Unit	Source
af	0.8291		Cheméo Relay (1.0)
gf	264.45	kJ/mol	Cheméo Relay (1.0, beta)
hf	99.26	kJ/mol	Cheméo Relay (1.0)
hvap	92.54	kJ/mol	Cheméo Relay (1.0)
ie	7.93	eV	Cheméo Relay (1.0)
log10ws	-6.11		Cheméo Relay (1.0)
logp	5.843		Crippen Method
mcvol	238.490	ml/mol	McGowan Method
pc	1487.29	kPa	Joback Method
tb	663.96	K	Cheméo Relay (1.0)
tc	870.58	K	Cheméo Relay (1.0)
tf	323.43	K	Cheméo Relay (1.0)
vc	0.884	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	535.00	J/mol×K	325.49	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31401340&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

af:	Acentric Factor
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

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