4,4'-Azobis(4-cyano-1-pentanol)

Inchi: InChI=1S/C12H20N4O2/c1-11(9-13,5-3-7-17)15-16-12(2,10-14)6-4-8-18/h17-18H,3-8H2
InchiKey: IWTIJBANDVIHPX-FOCLMDBBSA-N
Formula: C12H20N4O2
SMILES: CC(C#N)(CCCO)N=NC(C)(C#N)CCCO
Mol. weight [g/mol]: 252.31
CAS: 4693-47-4

Physical Properties

Property code	Value	Unit	Source
chs	-7357.10 ± 6.70	kJ/mol	NIST Webbook
hf	-235.99	kJ/mol	Joback Method
hfs	-223.30 ± 6.80	kJ/mol	NIST Webbook
hvap	100.70	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	1.548		Crippen Method
mcvol	210.100	ml/mol	McGowan Method
pc	1652.46	kPa	Joback Method
tb	1005.22	K	Joback Method
tc	1231.95	K	Joback Method

Sources

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=C4693474&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion

hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation 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