

4'-decyl[1,1'-biphenyl]-4-carbonitrile

Other names:	Decylcyanobiphenyl
Inchi:	InChI=1S/C23H29N/c1-2-3-4-5-6-7-8-9-10-20-11-15-22(16-12-20)23-17-13-21(19-24)14-
InchiKey:	GLGZJMAYDWXROS-UHFFFAOYSA-N
Formula:	C23H29N
SMILES:	CCCCCCCCCc1ccc(-c2ccc(C#N)cc2)cc1
Mol. weight [g/mol]:	319.48
CAS:	59454-35-2

Physical Properties

Property code	Value	Unit	Source
gf	481.52	kJ/mol	Joback Method
hf	96.95	kJ/mol	Joback Method
hfus	44.14	kJ/mol	Joback Method
hvap	83.15	kJ/mol	Joback Method
log10ws	-8.58		Crippen Method
logp	6.908		Crippen Method
mcvol	288.790	ml/mol	McGowan Method
pc	1258.37	kPa	Joback Method
tb	891.04	K	Joback Method
tc	1112.47	K	Joback Method
tf	491.84	K	Joback Method
vc	1.133	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	894.48	J/molxK	891.04	Joback Method
cpg	910.71	J/molxK	927.95	Joback Method
cpg	925.83	J/molxK	964.85	Joback Method
cpg	939.92	J/molxK	1001.76	Joback Method
cpg	953.05	J/molxK	1038.66	Joback Method
cpg	965.29	J/molxK	1075.57	Joback Method
cpg	976.74	J/molxK	1112.47	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C59454352&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
h vap:	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

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