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

Other names: 4-Nonyl-4'-cyanobiphenyl
Inchi: InChI=1S/C22H27N/c1-2-3-4-5-6-7-8-9-19-10-14-21(15-11-19)22-16-12-20(18-23)13-17-
InchiKey: REDSMJNHKIHBTE-UHFFFAOYSA-N
Formula: C22H27N
SMILES: CCCCCCCCCc1ccc(-c2ccc(C#N)cc2)cc1
Mol. weight [g/mol]: 305.46
CAS: 52709-85-0

Physical Properties

Property code	Value	Unit	Source
gf	473.10	kJ/mol	Joback Method
hf	117.59	kJ/mol	Joback Method
hfus	41.55	kJ/mol	Joback Method
hvap	80.92	kJ/mol	Joback Method
log10ws	-8.16		Crippen Method
logp	6.518		Crippen Method
mcvol	274.700	ml/mol	McGowan Method
pc	1348.67	kPa	Joback Method
tb	868.16	K	Joback Method
tc	1090.87	K	Joback Method
tf	313.70 ± 0.20	K	NIST Webbook
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.47	J/mol×K	868.16	Joback Method
cpg	851.54	J/mol×K	905.28	Joback Method
cpg	866.50	J/mol×K	942.40	Joback Method
cpg	880.41	J/mol×K	979.52	Joback Method
cpg	893.37	J/mol×K	1016.64	Joback Method
cpg	905.44	J/mol×K	1053.75	Joback Method
cpg	916.70	J/mol×K	1090.87	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=C52709850&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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