Decylcyanobiphenyl

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: CCCCCCCCCCc1ccc(-c2ccc(C#N)cc2)cc1
Mol. weight [g/mol]: 319.49

Physical Properties

Property code	Value	Unit	Source
af	0.8814		Cheméo Relay (1.0)
hfus	44.14	kJ/mol	Joback Method
hvap	122.97	kJ/mol	Cheméo Relay (1.0)
ie	8.97	eV	Cheméo Relay (1.0)
log10ws	-8.14		Cheméo Relay (1.0)
logp	6.908		Crippen Method
mcvol	288.790	ml/mol	McGowan Method
pc	1258.37	kPa	Joback Method
tb	703.43	K	Cheméo Relay (1.0)
tc	930.46	K	Cheméo Relay (1.0)
tf	318.00 ± 2.00	K	NIST Webbook
vc	1.082	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59454352&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
Cheméo Relay (1.0):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion 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