4-N-heptylbiphenyl

Other names: 1,1'-Biphenyl, 4-heptyl-
Inchi: InChI=1S/C19H24/c1-2-3-4-5-7-10-17-13-15-19(16-14-17)18-11-8-6-9-12-18/h6,8-9,11-1
InchiKey: KZIZPXDIBXXKAJ-UHFFFAOYSA-N
Formula: C19H24
SMILES: CCCCCCCc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 252.40

Physical Properties

Property code	Value	Unit	Source
af	0.6623		Cheméo Relay (1.0)
gf	324.29	kJ/mol	Joback Method
hf	47.01	kJ/mol	Cheméo Relay (1.0)
hfus	32.66	kJ/mol	Joback Method
hvap	93.53	kJ/mol	Cheméo Relay (1.0)
ie	8.24	eV	Cheméo Relay (1.0)
log10ws	-7.16		Cheméo Relay (1.0)
logp	5.866		Crippen Method
mcvol	231.050	ml/mol	McGowan Method
pc	1743.37	kPa	Joback Method
tb	634.26	K	Cheméo Relay (1.0)
tc	824.95	K	Cheméo Relay (1.0)
tf	296.69	K	Cheméo Relay (1.0)
vc	0.879	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.22	J/mol×K	692.46	Joback Method
cpg	730.03	J/mol×K	911.11	Joback Method
cpg	716.43	J/mol×K	874.67	Joback Method
cpg	701.85	J/mol×K	838.23	Joback Method
cpg	686.21	J/mol×K	801.78	Joback Method
cpg	669.43	J/mol×K	765.34	Joback Method
cpg	651.46	J/mol×K	728.90	Joback Method

dvisc	0.0002797	Pa×s	530.86	Joback Method
dvisc	0.0001104	Pa×s	692.46	Joback Method
dvisc	0.0001428	Pa×s	638.59	Joback Method
dvisc	0.0001938	Pa×s	584.72	Joback Method
dvisc	0.0015996	Pa×s	369.25	Joback Method
dvisc	0.0004387	Pa×s	476.99	Joback Method
dvisc	0.0007715	Pa×s	423.12	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59662327&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
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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