2,6-diethylnaphthalene

Inchi: InChI=1S/C14H16/c1-3-11-5-7-14-10-12(4-2)6-8-13(14)9-11/h5-10H,3-4H2,1-2H3
InchiKey: CJJFFBINNGWEBO-UHFFFAOYSA-N
Formula: C14H16
SMILES: CCc1ccc2cc(CC)ccc2c1
Mol. weight [g/mol]: 184.28
CAS: 59919-41-4

Physical Properties

Property code	Value	Unit	Source
af	0.5182		Cheméo Relay (1.0)
gf	266.80	kJ/mol	Joback Method
hf	57.03	kJ/mol	Cheméo Relay (1.0)
hfus	22.30	kJ/mol	Joback Method
hvap	74.64	kJ/mol	Cheméo Relay (1.0)
ie	7.82	eV	Cheméo Relay (1.0)
log10ws	-5.83		Cheméo Relay (1.0)
logp	3.965		Crippen Method
mcvol	164.900	ml/mol	McGowan Method
pc	2460.47	kPa	Joback Method
tb	565.60	K	Cheméo Relay (1.0)
tc	786.16	K	Cheméo Relay (1.0)
tf	336.48	K	Cheméo Relay (1.0)
vc	0.631	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.82	J/mol×K	575.34	Joback Method
cpg	406.19	J/mol×K	612.51	Joback Method
cpg	421.50	J/mol×K	649.68	Joback Method
cpg	435.82	J/mol×K	686.85	Joback Method
cpg	449.22	J/mol×K	724.03	Joback Method
cpg	461.76	J/mol×K	761.20	Joback Method
cpg	473.50	J/mol×K	798.37	Joback Method

dvisc	0.0013867	Pa×s	331.70	Joback Method
dvisc	0.0009157	Pa×s	372.31	Joback Method
dvisc	0.0006561	Pa×s	412.91	Joback Method
dvisc	0.0004990	Pa×s	453.52	Joback Method
dvisc	0.0003970	Pa×s	494.13	Joback Method
dvisc	0.0003270	Pa×s	534.73	Joback Method
dvisc	0.0002769	Pa×s	575.34	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55455e+01
Coeff. B	-5.02783e+03
Coeff. C	-1.01278e+02
Temperature range (K), min.	430.80
Temperature range (K), max.	592.56

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume