

2,6-Diisopropyl naphthalene

Other names:	2,6-Bis(1-methylethyl)naphthalene 2,6-diisopropyl naphthalene Diisopropyl naphthalene (DIPN) Naphthalene, 2,6-bis(1-methylethyl)- Naphthalene, 2,6-diisopropyl-
Inchi:	InChI=1S/C16H20/c1-11(2)13-5-7-16-10-14(12(3)4)6-8-15(16)9-13/h5-12H,1-4H3
InchiKey:	GWLLTEXUIOFAFE-UHFFFAOYSA-N
Formula:	C16H20
SMILES:	CC(C)c1ccc2cc(C(C)C)ccc2c1
Mol. weight [g/mol]:	212.34
CAS:	24157-81-1

Physical Properties

Property code	Value	Unit	Source
af	0.5077		Cheméo Relay (1.0)
gf	278.76	kJ/mol	Joback Method
hf	-16.65	kJ/mol	Cheméo Relay (1.0)
hfus	20.43	kJ/mol	Joback Method
hvap	79.59	kJ/mol	Cheméo Relay (1.0)
ie	7.80	eV	Cheméo Relay (1.0)
log10ws	-6.58		Cheméo Relay (1.0)
logp	5.087		Crippen Method
mcvol	193.080	ml/mol	McGowan Method
pc	2081.22	kPa	Joback Method
rinpol	1735.00		NIST Webbook
rinpol	1727.00		NIST Webbook
rinpol	1716.80		NIST Webbook
rinpol	1728.00		NIST Webbook
rinpol	1735.50		NIST Webbook
rinpol	1716.80		NIST Webbook
rinpol	1728.00		NIST Webbook
rinpol	1735.50		NIST Webbook
rinpol	1728.00		NIST Webbook
rinpol	1728.00		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1728.00		NIST Webbook
rinpol	1733.00		NIST Webbook

rinpol	1728.00		NIST Webbook
rinpol	1704.00		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1728.00		NIST Webbook
ripol	2242.00		NIST Webbook
ripol	2214.00		NIST Webbook
ripol	2242.00		NIST Webbook
tb	581.13	K	Cheméo Relay (1.0)
tc	809.58	K	Cheméo Relay (1.0)
tf	360.85	K	Cheméo Relay (1.0)
vc	0.725	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.58	J/mol×K	620.22	Joback Method
cpg	508.84	J/mol×K	657.59	Joback Method
cpg	525.92	J/mol×K	694.95	Joback Method
cpg	541.89	J/mol×K	732.32	Joback Method
cpg	556.83	J/mol×K	769.68	Joback Method
cpg	570.80	J/mol×K	807.05	Joback Method
cpg	583.89	J/mol×K	844.42	Joback Method
dvisc	0.0020223	Pa×s	324.24	Joback Method
dvisc	0.0010863	Pa×s	373.57	Joback Method
dvisc	0.0006746	Pa×s	422.90	Joback Method
dvisc	0.0004627	Pa×s	472.23	Joback Method
dvisc	0.0003409	Pa×s	521.56	Joback Method
dvisc	0.0002647	Pa×s	570.89	Joback Method
dvisc	0.0002140	Pa×s	620.22	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.18890e+01
Coeff. B	-3.63968e+03
Coeff. C	-9.47310e+01

Temperature range (K), min.	408.46
Temperature range (K), max.	648.09

Sources

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):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24157811&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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