1,3-di-iso-propylnaphthalene

Other names: Naphthalene, 1,3-diisopropyl
Inchi: InChI=1S/C16H20/c1-11(2)14-9-13-7-5-6-8-15(13)16(10-14)12(3)4/h5-12H,1-4H3
InchiKey: JDBFIFNXALGSOF-UHFFFAOYSA-N
Formula: C16H20
SMILES: CC(C)c1cc(C(C)C)c2ccccc2c1
Mol. weight [g/mol]: 212.33

Physical Properties

Property code	Value	Unit	Source
gf	278.76	kJ/mol	Joback Method
hf	20.53	kJ/mol	Joback Method
hfus	20.43	kJ/mol	Joback Method
hvap	55.67	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.087		Crippen Method
mcvol	193.080	ml/mol	McGowan Method
pc	2081.22	kPa	Joback Method
rinpol	1662.00		NIST Webbook
ripol	2162.00		NIST Webbook
ripol	2139.00		NIST Webbook
tb	620.22	K	Joback Method
tc	844.42	K	Joback Method
tf	324.24	K	Joback Method
vc	0.734	m3/kmol	Joback Method

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

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U374052&Units=SI

Legend

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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical 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