Naphthalene, 2-hexyl-

Inchi: InChI=1S/C16H20/c1-2-3-4-5-8-14-11-12-15-9-6-7-10-16(15)13-14/h6-7,9-13H,2-5,8H2,1
InchiKey: ZGHJVWFEQWVPTB-UHFFFAOYSA-N
Formula: C16H20
SMILES: CCCCCCc1ccc2ccccc2c1
Mol. weight [g/mol]: 212.33
CAS: 2876-46-2

Physical Properties

Property code	Value	Unit	Source
gf	293.27	kJ/mol	Joback Method
hf	42.56	kJ/mol	Joback Method
hfus	27.87	kJ/mol	Joback Method
hvap	55.79	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	4.963		Crippen Method
mcvol	193.080	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
tb	596.70 ± 3.00	K	NIST Webbook
tb	596.70 ± 3.00	K	NIST Webbook
tb	578.00 ± 8.00	K	NIST Webbook
tb	596.00 ± 5.00	K	NIST Webbook
tc	830.41	K	Joback Method
tf	267.60 ± 2.00	K	NIST Webbook
tf	266.30 ± 1.50	K	NIST Webbook
tf	280.00 ± 3.00	K	NIST Webbook
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.95	J/mol×K	616.12	Joback Method
cpg	507.63	J/mol×K	651.83	Joback Method
cpg	524.20	J/mol×K	687.55	Joback Method
cpg	539.72	J/mol×K	723.26	Joback Method

cpg	554.26	J/mol×K	758.98	Joback Method
cpg	567.91	J/mol×K	794.69	Joback Method
cpg	580.72	J/mol×K	830.41	Joback Method
dvisc	0.0017615	Pa×s	341.72	Joback Method
dvisc	0.0010486	Pa×s	387.45	Joback Method
dvisc	0.0006965	Pa×s	433.19	Joback Method
dvisc	0.0005002	Pa×s	478.92	Joback Method
dvisc	0.0003806	Pa×s	524.65	Joback Method
dvisc	0.0003026	Pa×s	570.39	Joback Method
dvisc	0.0002489	Pa×s	616.12	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol803.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2876462&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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