NAPHTHALENE, 1-ETHYL-1,2,3,4-TETRAHYDRO-

Other names: 1-Ethyltetralin
Tetraline, 1-ethyl

Inchi: InChI=1S/C12H16/c1-2-10-7-5-8-11-6-3-4-9-12(10)11/h3-4,6,9-10H,2,5,7-8H2,1H3

InchiKey: AXLCNVVQTVIXDG-UHFFFAOYSA-N

Formula: C12H16

SMILES: CCC1CCCc2ccccc21

Mol. weight [g/mol]: 160.26

Physical Properties

Property code	Value	Unit	Source
chl	-6920.80	kJ/mol	NIST Webbook
hfus	16.52	kJ/mol	Joback Method
ie	8.38	eV	Cheméo Relay (1.0)
logp	3.516		Crippen Method
mcvol	145.320	ml/mol	McGowan Method
rinpol	1308.09		NIST Webbook
rinpol	1321.92		NIST Webbook
rinpol	1337.31		NIST Webbook
rinpol	1324.00		NIST Webbook
rinpol	1324.00		NIST Webbook
rinpol	1293.93		NIST Webbook
rinpol	1337.31		NIST Webbook
rinpol	1331.29		NIST Webbook
rinpol	1302.33		NIST Webbook
rinpol	1293.93		NIST Webbook
tb	512.61 ± 0.15	K	NIST Webbook
tb	512.61 ± 0.15	K	NIST Webbook
tb	512.55 ± 0.40	K	NIST Webbook
tf	237.81	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.53	J/mol×K	516.63	Joback Method

cpg	351.20	J/mol×K	554.03	Joback Method
cpg	368.65	J/mol×K	591.44	Joback Method
cpg	384.96	J/mol×K	628.84	Joback Method
cpg	400.19	J/mol×K	666.24	Joback Method
cpg	414.40	J/mol×K	703.65	Joback Method
cpg	427.65	J/mol×K	741.05	Joback Method
dvisc	0.0021411	Pa×s	278.36	Joback Method
dvisc	0.0012955	Pa×s	318.07	Joback Method
dvisc	0.0008764	Pa×s	357.78	Joback Method
dvisc	0.0006410	Pa×s	397.50	Joback Method
dvisc	0.0004963	Pa×s	437.21	Joback Method
dvisc	0.0004009	Pa×s	476.92	Joback Method
dvisc	0.0003347	Pa×s	516.63	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13556586&Units=SI

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

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point