

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

Other names:	1-Propyltetralin
	Tetraline, 1-propyl
Inchi:	InChI=1S/C13H18/c1-2-6-11-8-5-9-12-7-3-4-10-13(11)12/h3-4,7,10-11H,2,5-6,8-9H2,1H3
InchiKey:	IXWKFZUCCCKIXFH-UHFFFAOYSA-N
Formula:	C13H18
SMILES:	CCCC1CCCC2CCCCC21
Mol. weight [g/mol]:	174.29

Physical Properties

Property code	Value	Unit	Source
hfus	19.11	kJ/mol	Joback Method
ie	8.33	eV	Cheméo Relay (1.0)
logp	3.907		Crippen Method
mcvol	159.410	ml/mol	McGowan Method
rinpol	1417.18		NIST Webbook
rinpol	1403.17		NIST Webbook
rinpol	1397.65		NIST Webbook
rinpol	1426.61		NIST Webbook
rinpol	1432.88		NIST Webbook
rinpol	1404.00		NIST Webbook
rinpol	1404.00		NIST Webbook
rinpol	1389.24		NIST Webbook
tb	529.36	K	Cheméo Relay (1.0)
tf	242.64	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.48	J/mol×K	539.51	Joback Method
cpg	479.11	J/mol×K	760.00	Joback Method
cpg	465.30	J/mol×K	723.26	Joback Method
cpg	450.53	J/mol×K	686.51	Joback Method
cpg	434.72	J/mol×K	649.76	Joback Method
cpg	417.82	J/mol×K	613.01	Joback Method

cpg	399.76	J/mol×K	576.26	Joback Method
dvisc	0.0006385	Pa×s	414.57	Joback Method
dvisc	0.0003240	Pa×s	539.51	Joback Method
dvisc	0.0003911	Pa×s	497.86	Joback Method
dvisc	0.0004887	Pa×s	456.22	Joback Method
dvisc	0.0022586	Pa×s	289.63	Joback Method
dvisc	0.0008855	Pa×s	372.92	Joback Method
dvisc	0.0013334	Pa×s	331.28	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C66324832&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

Cheméo Relay (1.0):

Legend

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

Latest version available from:

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