2-pentylnaphthalene

Inchi: InChI=1S/C15H18/c1-2-3-4-7-13-10-11-14-8-5-6-9-15(14)12-13/h5-6,8-12H,2-4,7H2,1H3
InchiKey: QCMRTPFHMFJUDP-UHFFFAOYSA-N
Formula: C15H18
SMILES: CCCCCc1ccc2ccccc2c1
Mol. weight [g/mol]: 198.30
CAS: 93-22-1

Physical Properties

Property code	Value	Unit	Source
af	0.5750		KDB
gf	284.85	kJ/mol	Joback Method
hf	63.20	kJ/mol	Joback Method
hfus	25.28	kJ/mol	Joback Method
hvap	53.56	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.572		Crippen Method
mcvol	178.990	ml/mol	McGowan Method
pc	2270.00	kPa	KDB
tb	583.00 ± 8.00	K	NIST Webbook
tb	583.00 ± 8.00	K	NIST Webbook
tb	566.20 ± 4.00	K	NIST Webbook
tb	581.00 ± 4.00	K	NIST Webbook
tb	565.50 ± 2.00	K	NIST Webbook
tb	583.20	K	KDB
tc	797.50	K	KDB
tf	259.10 ± 1.50	K	NIST Webbook
tf	269.00	K	KDB
tf	269.00 ± 3.00	K	NIST Webbook
vc	0.690	m3/kmol	KDB
zc	0.2360440		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	439.22	J/mol×K	593.24	Joback Method
cpg	514.89	J/mol×K	774.93	Joback Method
cpg	501.70	J/mol×K	738.59	Joback Method
cpg	487.61	J/mol×K	702.25	Joback Method
cpg	472.55	J/mol×K	665.92	Joback Method
cpg	456.44	J/mol×K	629.58	Joback Method
cpg	527.24	J/mol×K	811.27	Joback Method
dvisc	0.0002658	Pa×s	593.24	Joback Method
dvisc	0.0003212	Pa×s	549.44	Joback Method
dvisc	0.0004009	Pa×s	505.64	Joback Method
dvisc	0.0005221	Pa×s	461.85	Joback Method
dvisc	0.0007184	Pa×s	418.05	Joback Method
dvisc	0.0010653	Pa×s	374.25	Joback Method
dvisc	0.0017537	Pa×s	330.45	Joback Method

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol798.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93221&Units=SI
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

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
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
zc:	Critical Compressibility

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