

1-Isopropyl-8-methylnaphthalene

Inchi: InChI=1S/C14H16/c1-10(2)13-9-5-8-12-7-4-6-11(3)14(12)13/h4-10H,1-3H3
InchiKey: QEYRQUMIIMIEPQ-UHFFFAOYSA-N
Formula: C14H16
SMILES: Cc1cccc2cccc(C(C)C)c12
Mol. weight [g/mol]: 184.28
CAS: 81603-44-3

Physical Properties

Property code	Value	Unit	Source
chl	-7798.60 ± 1.00	kJ/mol	NIST Webbook
gf	264.36	kJ/mol	Joback Method
hf	67.09	kJ/mol	Joback Method
hfl	2.90 ± 1.30	kJ/mol	NIST Webbook
hfus	18.78	kJ/mol	Joback Method
hvap	51.61	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.272		Crippen Method
mcvol	164.900	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
tb	574.90	K	Joback Method
tc	802.86	K	Joback Method
tf	316.70	K	Joback Method
vc	0.627	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.19	J/mol×K	574.90	Joback Method
cpg	406.98	J/mol×K	612.89	Joback Method
cpg	422.66	J/mol×K	650.89	Joback Method
cpg	437.29	J/mol×K	688.88	Joback Method
cpg	450.95	J/mol×K	726.87	Joback Method
cpg	463.70	J/mol×K	764.87	Joback Method
cpg	475.62	J/mol×K	802.86	Joback Method

dvisc	0.0016365	Paxs	316.70	Joback Method
dvisc	0.0010016	Paxs	359.73	Joback Method
dvisc	0.0006808	Paxs	402.77	Joback Method
dvisc	0.0004986	Paxs	445.80	Joback Method
dvisc	0.0003857	Paxs	488.83	Joback Method
dvisc	0.0003110	Paxs	531.87	Joback Method
dvisc	0.0002590	Paxs	574.90	Joback Method

Sources

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=C81603443&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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

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