isopropylnaphthalene

Other names: isopropylnaphthalene
Inchi: InChI=1S/C13H14/c1-10(2)12-9-5-7-11-6-3-4-8-13(11)12/h3-10H,1-2H3
InchiKey: PMPBFICDXLLSRM-UHFFFAOYSA-N
Formula: C13H14
SMILES: CC(C)c1cccc2ccccc12
Mol. weight [g/mol]: 170.26

Physical Properties

Property code	Value	Unit	Source
af	0.4057		Cheméo Relay (1.0)
gf	265.57	kJ/mol	Joback Method
hf	66.92	kJ/mol	Cheméo Relay (1.0)
hfus	16.57	kJ/mol	Joback Method
hvap	67.45	kJ/mol	Cheméo Relay (1.0)
ie	7.99	eV	Cheméo Relay (1.0)
log10ws	-4.86		Cheméo Relay (1.0)
logp	3.963		Crippen Method
mcvol	150.810	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
rinpol	248.90		NIST Webbook
tb	541.30 ± 0.40	K	NIST Webbook
tc	775.90	K	Cheméo Relay (1.0)
tf	284.16	K	Cheméo Relay (1.0)
vc	0.563	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.66	J/mol×K	547.04	Joback Method
cpg	359.12	J/mol×K	585.59	Joback Method
cpg	374.41	J/mol×K	624.14	Joback Method
cpg	388.61	J/mol×K	662.69	Joback Method
cpg	401.80	J/mol×K	701.24	Joback Method
cpg	414.06	J/mol×K	739.79	Joback Method

cpg	425.45	J/mol×K	778.34	Joback Method
dvisc	0.0020244	Pa×s	292.91	Joback Method
dvisc	0.0011772	Pa×s	335.26	Joback Method
dvisc	0.0007731	Pa×s	377.62	Joback Method
dvisc	0.0005526	Pa×s	419.98	Joback Method
dvisc	0.0004201	Pa×s	462.33	Joback Method
dvisc	0.0003344	Pa×s	504.68	Joback Method
dvisc	0.0002758	Pa×s	547.04	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C29253369&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

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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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