Naphthalene, 1-(2-methylpropyl)-

Other names: Naphthalene, 1-isobutyl-
«alpha»-Isobutylnaphthalene
Inchi: InChI=1S/C14H16/c1-11(2)10-13-8-5-7-12-6-3-4-9-14(12)13/h3-9,11H,10H2,1-2H3
InchiKey: ZYFTVCJVNRKBCC-UHFFFAOYSA-N
Formula: C14H16
SMILES: CC(C)Cc1cccc2ccccc12
Mol. weight [g/mol]: 184.28
CAS: 16727-91-6

Physical Properties

Property code	Value	Unit	Source
gf	273.99	kJ/mol	Joback Method
hf	78.56	kJ/mol	Joback Method
hfus	19.16	kJ/mol	Joback Method
hvap	50.95	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.038		Crippen Method
mcvol	164.900	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
rinpol	1501.00		NIST Webbook
rinpol	1501.00		NIST Webbook
tb	552.49 ± 0.30	K	NIST Webbook
tc	796.83	K	Joback Method
tf	251.01 ± 0.40	K	NIST Webbook
tf	263.78 ± 0.20	K	NIST Webbook
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.34	J/mol×K	569.92	Joback Method
cpg	407.45	J/mol×K	607.74	Joback Method
cpg	423.38	J/mol×K	645.56	Joback Method
cpg	438.22	J/mol×K	683.37	Joback Method

cpg	452.03	J/mol×K	721.19	Joback Method
cpg	464.90	J/mol×K	759.01	Joback Method
cpg	476.91	J/mol×K	796.83	Joback Method
dvisc	0.0020876	Pa×s	304.18	Joback Method
dvisc	0.0011870	Pa×s	348.47	Joback Method
dvisc	0.0007666	Pa×s	392.76	Joback Method
dvisc	0.0005410	Pa×s	437.05	Joback Method
dvisc	0.0004070	Pa×s	481.34	Joback Method
dvisc	0.0003213	Pa×s	525.63	Joback Method
dvisc	0.0002631	Pa×s	569.92	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16727916&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

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
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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