1-Isopropyl-6-methylindane

Inchi: InChI=1S/C13H18/c1-9(2)12-7-6-11-5-4-10(3)8-13(11)12/h4-5,8-9,12H,6-7H2,1-3H3
InchiKey: VTHXZGHOXXVVSE-UHFFFAOYSA-N
Formula: C13H18
SMILES: Cc1ccc2c(c1)C(C(C)C)CC2
Mol. weight [g/mol]: 174.28
CAS: 828-97-7

Physical Properties

Property code	Value	Unit	Source
chl	-7574.30 ± 1.10	kJ/mol	NIST Webbook
gf	210.04	kJ/mol	Joback Method
hf	-30.54	kJ/mol	Joback Method
hfl	-113.00 ± 1.30	kJ/mol	NIST Webbook
hfus	17.30	kJ/mol	Joback Method
hvap	47.66	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.681		Crippen Method
mcvol	159.410	ml/mol	McGowan Method
pc	2433.84	kPa	Joback Method
tb	539.78	K	Joback Method
tc	758.37	K	Joback Method
tf	290.67	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.42	J/mol×K	539.78	Joback Method
cpg	398.79	J/mol×K	576.21	Joback Method
cpg	416.03	J/mol×K	612.64	Joback Method
cpg	432.20	J/mol×K	649.07	Joback Method
cpg	447.36	J/mol×K	685.51	Joback Method
cpg	461.58	J/mol×K	721.94	Joback Method
cpg	474.91	J/mol×K	758.37	Joback Method

dvisc	0.0017833	Pa×s	290.67	Joback Method
dvisc	0.0011663	Pa×s	332.19	Joback Method
dvisc	0.0008383	Pa×s	373.71	Joback Method
dvisc	0.0006437	Pa×s	415.23	Joback Method
dvisc	0.0005186	Pa×s	456.74	Joback Method
dvisc	0.0004331	Pa×s	498.26	Joback Method
dvisc	0.0003718	Pa×s	539.78	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C828977&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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