

1-Isopropyl-4-methylbicyclo[3.1.0]hexane

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C10H18/c1-7(2)10-5-4-8(3)9(10)6-10/h7-9H,4-6H2,1-3H3

GCTNBVHDRFKLLK-UHFFFAOYSA-N

C10H18

CC1CCC2(C(C)C)CC12

138.25

Physical Properties

Property code	Value	Unit	Source
gf	139.18	kJ/mol	Joback Method
hf	-114.51	kJ/mol	Joback Method
hfus	9.18	kJ/mol	Joback Method
hvap	35.83	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	3.079		Crippen Method
mcvol	130.040	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
tb	436.81	K	Joback Method
tc	639.14	K	Joback Method
tf	243.00	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.61	J/mol×K	436.81	Joback Method
cpg	307.00	J/mol×K	470.53	Joback Method
cpg	324.96	J/mol×K	504.25	Joback Method
cpg	341.63	J/mol×K	537.97	Joback Method
cpg	357.14	J/mol×K	571.70	Joback Method
cpg	371.61	J/mol×K	605.42	Joback Method
cpg	385.18	J/mol×K	639.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6004990&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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

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