

1,3-Diisopropyl cyclohexane

Inchi:	InChI=1S/C12H24/c1-9(2)11-6-5-7-12(8-11)10(3)4/h9-12H,5-8H2,1-4H3
InchiKey:	WDTCMYUFBNCSSK-UHFFFAOYSA-N
Formula:	C12H24
SMILES:	CC(C)C1CCCC(C(C)C)C1
Mol. weight [g/mol]:	168.32
CAS:	7045-70-7

Physical Properties

Property code	Value	Unit	Source
gf	62.02	kJ/mol	Joback Method
hf	-267.59	kJ/mol	Joback Method
hfus	12.70	kJ/mol	Joback Method
hvap	41.65	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	4.105		Crippen Method
mcvol	169.080	ml/mol	McGowan Method
pc	2100.34	kPa	Joback Method
tb	487.96	K	Joback Method
tc	688.60	K	Joback Method
tf	198.14	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.15	J/molxK	487.96	Joback Method
cpg	417.54	J/molxK	521.40	Joback Method
cpg	438.85	J/molxK	554.84	Joback Method
cpg	459.10	J/molxK	588.28	Joback Method
cpg	478.31	J/molxK	621.72	Joback Method
cpg	496.51	J/molxK	655.16	Joback Method
cpg	513.72	J/molxK	688.60	Joback Method
dvisc	0.0144098	Paxs	198.14	Joback Method
dvisc	0.0036341	Paxs	246.44	Joback Method

dvisc	0.0014395	Paxs	294.75	Joback Method
dvisc	0.0007401	Paxs	343.05	Joback Method
dvisc	0.0004484	Paxs	391.35	Joback Method
dvisc	0.0003033	Paxs	439.66	Joback Method
dvisc	0.0002217	Paxs	487.96	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=C7045707&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	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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