

1,3-Diisopropylcyclohexane

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

Physical Properties

Property code	Value	Unit	Source
af	0.3341		Cheméo Relay (1.0)
hf	-240.77	kJ/mol	Cheméo Relay (1.0)
hfus	12.70	kJ/mol	Joback Method
hvap	54.12	kJ/mol	Cheméo Relay (1.0)
ie	9.13	eV	Cheméo Relay (1.0)
logp	4.105		Crippen Method
mcvol	169.080	ml/mol	McGowan Method
pc	2100.34	kPa	Joback Method
tb	481.64	K	Cheméo Relay (1.0)
tc	675.03	K	Cheméo Relay (1.0)
tf	214.70	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.15	J/mol×K	487.96	Joback Method
cpg	417.54	J/mol×K	521.40	Joback Method
cpg	438.85	J/mol×K	554.84	Joback Method
cpg	459.10	J/mol×K	588.28	Joback Method
cpg	478.31	J/mol×K	621.72	Joback Method
cpg	496.51	J/mol×K	655.16	Joback Method
cpg	513.72	J/mol×K	688.60	Joback Method
dvisc	0.0144098	Pa×s	198.14	Joback Method
dvisc	0.0036341	Pa×s	246.44	Joback Method
dvisc	0.0014395	Pa×s	294.75	Joback Method
dvisc	0.0007401	Pa×s	343.05	Joback Method

dvisc	0.0004484	Pa×s	391.35	Joback Method
dvisc	0.0003033	Pa×s	439.66	Joback Method
dvisc	0.0002217	Pa×s	487.96	Joback Method

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7045707&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

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