

CYCLOHEXANE, (1-METHYLBUTYL)-

Other names:	2-cyclohexylpentane
Inchi:	InChI=1S/C11H22/c1-3-7-10(2)11-8-5-4-6-9-11/h10-11H,3-9H2,1-2H3
InchiKey:	ZYJFJURMFHCWOB-UHFFFAOYSA-N
Formula:	C11H22
SMILES:	CCCC(C)C1CCCCC1
Mol. weight [g/mol]:	154.30

Physical Properties

Property code	Value	Unit	Source
af	0.3299		Cheméo Relay (1.0)
hf	-213.23	kJ/mol	Cheméo Relay (1.0)
hfus	12.56	kJ/mol	Joback Method
hvap	50.23	kJ/mol	Cheméo Relay (1.0)
ie	9.52	eV	Cheméo Relay (1.0)
logp	4.003		Crippen Method
mcvol	154.990	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
tb	470.30	K	Cheméo Relay (1.0)
tc	664.43	K	Cheméo Relay (1.0)
tf	192.32	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.68	J/mol×K	470.19	Joback Method
cpg	367.48	J/mol×K	503.36	Joback Method
cpg	387.26	J/mol×K	536.52	Joback Method
cpg	406.04	J/mol×K	569.69	Joback Method
cpg	423.85	J/mol×K	602.85	Joback Method
cpg	440.74	J/mol×K	636.02	Joback Method
cpg	456.71	J/mol×K	669.19	Joback Method
dvisc	0.0145054	Pa×s	206.11	Joback Method
dvisc	0.0040021	Pa×s	250.12	Joback Method
dvisc	0.0016233	Pa×s	294.14	Joback Method

dvisc	0.0008328	Pa×s	338.15	Joback Method
dvisc	0.0004983	Pa×s	382.16	Joback Method
dvisc	0.0003315	Pa×s	426.18	Joback Method
dvisc	0.0002380	Pa×s	470.19	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C61208944&Units=SI>

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

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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