

CYCLOHEXANE, CYCLOHEXYLIDENE-

Inchi: InChI=1S/C12H20/c1-3-7-11(8-4-1)12-9-5-2-6-10-12/h1-10H2
InchiKey: FJHVMZDLYBHASM-UHFFFAOYSA-N
Formula: C12H20
SMILES: C1CCC(=C2CCCCC2)CC1
Mol. weight [g/mol]: 164.29

Physical Properties

Property code	Value	Unit	Source
af	0.2873		Cheméo Relay (1.0)
gf	125.18	kJ/mol	Joback Method
hf	-83.24	kJ/mol	Cheméo Relay (1.0)
hfus	8.81	kJ/mol	Joback Method
hvap	59.04	kJ/mol	Cheméo Relay (1.0)
ie	8.16 ± 0.02	eV	NIST Webbook
log10ws	-4.58		Cheméo Relay (1.0)
logp	4.211		Crippen Method
mcvol	153.920	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
tb	510.72	K	Cheméo Relay (1.0)
tc	724.43	K	Cheméo Relay (1.0)
tf	300.84	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.14	J/mol×K	531.52	Joback Method
cpg	392.10	J/mol×K	571.03	Joback Method
cpg	413.56	J/mol×K	610.54	Joback Method
cpg	433.59	J/mol×K	650.05	Joback Method
cpg	452.24	J/mol×K	689.56	Joback Method
cpg	469.58	J/mol×K	729.07	Joback Method
cpg	485.67	J/mol×K	768.58	Joback Method
dvisc	0.0066760	Pa×s	274.04	Joback Method
dvisc	0.0025025	Pa×s	316.95	Joback Method

dvisc	0.0011854	Pa×s	359.87	Joback Method
dvisc	0.0006584	Pa×s	402.78	Joback Method
dvisc	0.0004096	Pa×s	445.69	Joback Method
dvisc	0.0002769	Pa×s	488.61	Joback Method
dvisc	0.0001995	Pa×s	531.52	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C4233185&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
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
ie:	Ionization energy
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

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