

Cyclohexane, 1-ethyl-2,3-dimethyl-

Inchi:	InChI=1S/C10H20/c1-4-10-7-5-6-8(2)9(10)3/h8-10H,4-7H2,1-3H3
InchiKey:	VJIJHYHFBLLMQS-UHFFFAOYSA-N
Formula:	C10H20
SMILES:	CCC1CCCC(C)C1C
Mol. weight [g/mol]:	140.27
CAS:	7058-05-1

Physical Properties

Property code	Value	Unit	Source
gf	42.35	kJ/mol	Joback Method
hf	-236.09	kJ/mol	Joback Method
hfus	15.63	kJ/mol	Joback Method
hvap	37.67	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	3.469		Crippen Method
mcvol	140.900	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
tb	438.41	K	Joback Method
tc	634.46	K	Joback Method
tf	201.36	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.43	J/mol×K	438.41	Joback Method
cpg	391.37	J/mol×K	601.79	Joback Method
cpg	374.66	J/mol×K	569.11	Joback Method
cpg	357.12	J/mol×K	536.44	Joback Method
cpg	338.75	J/mol×K	503.76	Joback Method
cpg	319.52	J/mol×K	471.09	Joback Method
cpg	407.27	J/mol×K	634.46	Joback Method
dvisc	0.0002623	Pa×s	438.41	Joback Method
dvisc	0.0003200	Pa×s	398.90	Joback Method

dvisc	0.0004080	Pa×s	359.39	Joback Method
dvisc	0.0005522	Pa×s	319.88	Joback Method
dvisc	0.0008141	Pa×s	280.38	Joback Method
dvisc	0.0013629	Pa×s	240.87	Joback Method
dvisc	0.0027933	Pa×s	201.36	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=C7058051&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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