

Cyclohexene, 3,6-dimethyl-, trans

Inchi:	InChI=1S/C8H14/c1-7-3-5-8(2)6-4-7/h3,5,7-8H,4,6H2,1-2H3/t7-,8-/m0/s1
InchiKey:	ADPYSZNUBWNLDH-YUMQZZPRSA-N
Formula:	C8H14
SMILES:	CC1C=CC(C)CC1
Mol. weight [g/mol]:	110.20

Physical Properties

Property code	Value	Unit	Source
gf	63.18	kJ/mol	Joback Method
hf	-116.69	kJ/mol	Joback Method
hfus	10.60	kJ/mol	Joback Method
hvap	33.81	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	2.609		Crippen Method
mcvol	108.420	ml/mol	McGowan Method
pc	3163.27	kPa	Joback Method
ripol	910.00		NIST Webbook
ripol	910.00		NIST Webbook
tb	396.48	K	Joback Method
tc	598.94	K	Joback Method
tf	183.82	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.92	J/mol×K	396.48	Joback Method
cpg	274.86	J/mol×K	565.20	Joback Method
cpg	261.33	J/mol×K	531.46	Joback Method
cpg	247.09	J/mol×K	497.71	Joback Method
cpg	232.12	J/mol×K	463.97	Joback Method
cpg	216.40	J/mol×K	430.22	Joback Method
cpg	287.70	J/mol×K	598.94	Joback Method
dvisc	0.0002471	Pa×s	396.48	Joback Method

dvisc	0.0003046	Pa×s	361.04	Joback Method
dvisc	0.0003929	Pa×s	325.59	Joback Method
dvisc	0.0005394	Pa×s	290.15	Joback Method
dvisc	0.0008088	Pa×s	254.71	Joback Method
dvisc	0.0013823	Pa×s	219.26	Joback Method
dvisc	0.0029050	Pa×s	183.82	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=R297433&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log_{10ws}:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
ri_{pol}:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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