trans-3,6-dimethylcyclohexene

Other names: cis-3,6-dimethylcyclohexene
Cyclohexene, 3,6-dimethyl-, cis
Cyclohexene, 3,6-dimethyl-
Inchi: InChI=1S/C8H14/c1-7-3-5-8(2)6-4-7/h3,5,7-8H,4,6H2,1-2H3
InchiKey: ADPYSZNUBWNLDH-UHFFFAOYSA-N
Formula: C8H14
SMILES: CC1C=CC(C)CC1
Mol. weight [g/mol]: 110.20
CAS: 19550-40-4

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
rinpol	790.80		NIST Webbook
rinpol	779.30		NIST Webbook
rinpol	795.50		NIST Webbook
rinpol	789.80		NIST Webbook
ripol	924.00		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	216.40	J/mol×K	430.22	Joback Method
cpg	232.12	J/mol×K	463.97	Joback Method
cpg	247.09	J/mol×K	497.71	Joback Method
cpg	261.33	J/mol×K	531.46	Joback Method
cpg	274.86	J/mol×K	565.20	Joback Method
cpg	287.70	J/mol×K	598.94	Joback Method
dvisc	0.0029050	Pa×s	183.82	Joback Method
dvisc	0.0013823	Pa×s	219.26	Joback Method
dvisc	0.0008088	Pa×s	254.71	Joback Method
dvisc	0.0005394	Pa×s	290.15	Joback Method
dvisc	0.0003929	Pa×s	325.59	Joback Method
dvisc	0.0003046	Pa×s	361.04	Joback Method
dvisc	0.0002471	Pa×s	396.48	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=C19550404&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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume