cis-1,3,5-trimethylcyclohexene

Inchi: InChI=1S/C9H18/c1-7-4-8(2)6-9(3)5-7/h7-9H,4-6H2,1-3H3
InchiKey: ODNRTOSCFYDTKF-AYMMMOKOSA-N
Formula: C9H16
SMILES: CC1CC(C)CC(C)C1
Mol. weight [g/mol]: 124.22
CAS: 24583-97-9

Physical Properties

Property code	Value	Unit	Source
af	0.2881		Cheméo Relay (1.0)
gf	33.93	kJ/mol	Joback Method
hf	-218.31	kJ/mol	Cheméo Relay (1.0)
hfus	13.04	kJ/mol	Joback Method
hvap	40.96	kJ/mol	Cheméo Relay (1.0)
ie	9.30	eV	Cheméo Relay (1.0)
log10ws	-5.15		Cheméo Relay (1.0)
logp	3.079		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method
tb	415.10 ± 0.60	K	NIST Webbook
tc	587.59	K	Cheméo Relay (1.0)
tf	185.70 ± 0.30	K	NIST Webbook
vc	0.458	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.82	J/mol×K	415.53	Joback Method
cpg	273.92	J/mol×K	448.54	Joback Method
cpg	292.21	J/mol×K	481.54	Joback Method
cpg	309.72	J/mol×K	514.55	Joback Method
cpg	326.43	J/mol×K	547.56	Joback Method
cpg	342.37	J/mol×K	580.57	Joback Method
cpg	357.55	J/mol×K	613.57	Joback Method

dvisc	0.0024227	Pa×s	190.09	Joback Method
dvisc	0.0012236	Pa×s	227.66	Joback Method
dvisc	0.0007500	Pa×s	265.24	Joback Method
dvisc	0.0005190	Pa×s	302.81	Joback Method
dvisc	0.0003896	Pa×s	340.38	Joback Method
dvisc	0.0003096	Pa×s	377.96	Joback Method
dvisc	0.0002565	Pa×s	415.53	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24583979&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
vc: Critical Volume

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