Cyclohexene, 1,4,5-trimethyl-

Other names: 1,4,5-trimethylcyclohexene
Inchi: InChI=1S/C9H16/c1-7-4-5-8(2)9(3)6-7/h4,8-9H,5-6H2,1-3H3
InchiKey: FNZUANSNHGITHR-UHFFFAOYSA-N
Formula: C9H16
SMILES: CC1=CCC(C)C(C)C1
Mol. weight [g/mol]: 124.22
CAS: 20030-32-4

Physical Properties

Property code	Value	Unit	Source
gf	61.97	kJ/mol	Joback Method
hf	-148.80	kJ/mol	Joback Method
hfus	12.80	kJ/mol	Joback Method
hvap	36.70	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.999		Crippen Method
mcvol	122.510	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
rinpol	908.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	908.00		NIST Webbook
tb	418.00 ± 5.00	K	NIST Webbook
tc	626.38	K	Joback Method
tf	207.61	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.33	J/mol×K	424.34	Joback Method
cpg	321.55	J/mol×K	592.70	Joback Method
cpg	307.37	J/mol×K	559.03	Joback Method
cpg	292.47	J/mol×K	525.36	Joback Method
cpg	276.84	J/mol×K	491.69	Joback Method

cpg	260.46	J/mol×K	458.01	Joback Method
cpg	335.03	J/mol×K	626.38	Joback Method
dvisc	0.0002413	Pa×s	424.34	Joback Method
dvisc	0.0002931	Pa×s	388.22	Joback Method
dvisc	0.0003706	Pa×s	352.10	Joback Method
dvisc	0.0004943	Pa×s	315.98	Joback Method
dvisc	0.0007103	Pa×s	279.85	Joback Method
dvisc	0.0011365	Pa×s	243.73	Joback Method
dvisc	0.0021413	Pa×s	207.61	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44487e+01
Coeff. B	-3.54486e+03
Coeff. C	-5.73960e+01
Temperature range (K), min.	307.72
Temperature range (K), max.	445.36

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C20030324&Units=SI

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume