Cyclohexene, 3,5,5-trimethyl-

Other names: 3,5,5-Trimethylcyclohexene
«delta»-Cyclogeraniolene
Â«deltaÂ»-Cyclogeraniolene
Inchi: InChI=1S/C9H16/c1-8-5-4-6-9(2,3)7-8/h4-5,8H,6-7H2,1-3H3
InchiKey: CBERVMGFVLWZSU-UHFFFAOYSA-N
Formula: C9H16
SMILES: CC1C=CCC(C)(C)C1
Mol. weight [g/mol]: 124.22
CAS: 933-12-0

Physical Properties

Property code	Value	Unit	Source
gf	66.11	kJ/mol	Joback Method
hf	-122.09	kJ/mol	Joback Method
hfus	6.90	kJ/mol	Joback Method
hvap	34.89	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.999		Crippen Method
mcvol	122.510	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
rinpol	1182.00		NIST Webbook
rinpol	1182.00		NIST Webbook
tb	406.73 ± 0.30	K	NIST Webbook
tb	406.73 ± 0.30	K	NIST Webbook
tb	406.76 ± 0.20	K	NIST Webbook
tc	629.34	K	Joback Method
tf	181.18 ± 0.30	K	NIST Webbook
tf	181.90 ± 0.20	K	NIST Webbook
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.29	J/mol×K	419.60	Joback Method

cpg	260.61	J/mol×K	454.56	Joback Method
cpg	277.72	J/mol×K	489.51	Joback Method
cpg	293.72	J/mol×K	524.47	Joback Method
cpg	308.70	J/mol×K	559.43	Joback Method
cpg	322.78	J/mol×K	594.39	Joback Method
cpg	336.03	J/mol×K	629.34	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44031e+01
Coeff. B	-3.44945e+03
Coeff. C	-5.42260e+01
Temperature range (K), min.	298.60
Temperature range (K), max.	433.64

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=C933120&Units=SI

Legend

cpg: Ideal gas heat capacity
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