Cyclohexene, 3,3,5-trimethyl-

Other names: «epsilon»-Cyclogeraniolene
3,3,5-Trimethylcyclohexene
3,5,5-Trimethyl-1-cyclohexene
3,3,5-Trimethyl-1-cyclohexene
Inchi: InChI=1S/C9H16/c1-8-5-4-6-9(2,3)7-8/h4,6,8H,5,7H2,1-3H3
InchiKey: GQVLBFQEABXQDC-UHFFFAOYSA-N
Formula: C9H16
SMILES: CC1CC=CC(C)(C)C1
Mol. weight [g/mol]: 124.22
CAS: 503-45-7

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
ripol	1633.00		NIST Webbook
tb	404.44 ± 0.20	K	NIST Webbook
tb	404.48 ± 0.20	K	NIST Webbook
tc	629.34	K	Joback Method
tf	187.76 ± 0.30	K	NIST Webbook
tf	187.91 ± 0.30	K	NIST Webbook
tf	187.72 ± 0.30	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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C503457&Units=SI
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume