

Cyclohexene, 1,4,4-trimethyl-

Inchi:	InChI=1S/C9H16/c1-8-4-6-9(2,3)7-5-8/h4H,5-7H2,1-3H3
InchiKey:	VUWMEDZMVLUYQB-UHFFFAOYSA-N
Formula:	C9H16
SMILES:	CC1=CCC(C)(C)CC1
Mol. weight [g/mol]:	124.22
CAS:	3419-71-4

Physical Properties

Property code	Value	Unit	Source
gf	64.19	kJ/mol	Joback Method
hf	-113.22	kJ/mol	Joback Method
hfus	5.44	kJ/mol	Joback Method
hvap	35.86	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	3.143		Crippen Method
mvol	122.510	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
rinpol	887.00		NIST Webbook
rinpol	887.00		NIST Webbook
tb	413.20	K	NIST Webbook
tc	640.93	K	Joback Method
tf	235.75	K	Joback Method
vc	0.457	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.07	J/molxK	429.25	Joback Method
cpg	261.48	J/molxK	464.53	Joback Method
cpg	277.72	J/molxK	499.81	Joback Method
cpg	292.91	J/molxK	535.09	Joback Method
cpg	307.14	J/molxK	570.37	Joback Method
cpg	320.51	J/molxK	605.65	Joback Method
cpg	333.12	J/molxK	640.93	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	310.50	K	1.90	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3419714&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

Latest version available from:

<https://www.cheméo.com/cid/19-240-4/Cyclohexene-1-4-4-trimethyl.pdf>

Generated by Cheméo on 2024-04-18 07:33:31.456123355 +0000 UTC m=+15714860.376700711.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.