

Cyclopentane, 1,2,4-trimethyl-

Other names:	1,2,4-Trimethylcyclopentane
Inchi:	InChI=1S/C8H16/c1-6-4-7(2)8(3)5-6/h6-8H,4-5H2,1-3H3/t7-,8-/m0/s1
InchiKey:	PNUFYSGVPVMNRN-YUMQZZPRSA-N
Formula:	C8H16
SMILES:	CC1CC(C)C(C)C1
Mol. weight [g/mol]:	112.21
CAS:	2815-58-9

Physical Properties

Property code	Value	Unit	Source
gf	37.61	kJ/mol	Joback Method
hf	-188.65	kJ/mol	Joback Method
hfus	12.55	kJ/mol	Joback Method
hvap	33.04	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	2.688		Crippen Method
mcvol	112.720	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	777.10		NIST Webbook
rinpol	797.00		NIST Webbook
rinpol	742.30		NIST Webbook
rinpol	742.40		NIST Webbook
rinpol	741.00		NIST Webbook
rinpol	760.00		NIST Webbook
rinpol	741.00		NIST Webbook
rinpol	741.00		NIST Webbook
rinpol	740.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	743.00		NIST Webbook
rinpol	771.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	740.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	759.00		NIST Webbook
tb	388.38	K	Joback Method
tc	579.97	K	Joback Method

tf	182.34	K	Joback Method
vc	0.422	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.62	J/mol×K	388.38	Joback Method
cpg	230.52	J/mol×K	420.31	Joback Method
cpg	246.72	J/mol×K	452.24	Joback Method
cpg	262.24	J/mol×K	484.17	Joback Method
cpg	277.08	J/mol×K	516.11	Joback Method
cpg	291.26	J/mol×K	548.04	Joback Method
cpg	304.79	J/mol×K	579.97	Joback Method
dvisc	0.0010560	Pa×s	182.34	Joback Method
dvisc	0.0006962	Pa×s	216.68	Joback Method
dvisc	0.0005145	Pa×s	251.02	Joback Method
dvisc	0.0004089	Pa×s	285.36	Joback Method
dvisc	0.0003414	Pa×s	319.70	Joback Method
dvisc	0.0002952	Pa×s	354.04	Joback Method
dvisc	0.0002619	Pa×s	388.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2815589&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

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

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