Cyclopentane, 1,2,3-trimethyl-, (1«alpha»,2«alpha»,3«beta»)-

Other names: 1,2,3-Trimethylcyclopentane, cis, trans
1,2,3-Trimethylcyclopentane, trans, cis
1,trans-2,cis-3-Trimethylcyclopentane
1-cis-2, trans-3-Trimethylcyclopentane
Cyclopentane, 1,2,3-trimethyl-, cis,trans
Cyclopentane, 1,2,3-trimethyl-, cis-1,2,trans-1,3-
Cyclopentane, 1,2,3-trimethyl-, trans, cis
cis 1,2-trans-3-trimethylcyclopentane
trans,cis-1,2,3-Trimethylcyclopentane

Inchi: InChI=1S/C8H16/c1-6-4-5-7(2)8(6)3/h6-8H,4-5H2,1-3H3/t6-,7-/m1/s1

InchiKey: VCWNHOPGKQCXIQ-RNFRBKRXSA-N

Formula: C8H16

SMILES: CC1CCC(C)C1C

Mol. weight [g/mol]: 112.21

CAS: 15890-40-1

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	38.10	kJ/mol	NIST Webbook
log10ws	-2.34		Crippen Method
logp	2.688		Crippen Method
mcvol	112.720	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	753.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	738.00		NIST Webbook
rinpol	750.80		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	772.70		NIST Webbook
rinpol	777.90		NIST Webbook
rinpol	782.70		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	748.00		NIST Webbook

rinpol	750.00	NIST Webbook
rinpol	745.30	NIST Webbook
rinpol	747.10	NIST Webbook
rinpol	748.90	NIST Webbook
rinpol	750.90	NIST Webbook
rinpol	747.80	NIST Webbook
rinpol	778.80	NIST Webbook
rinpol	742.00	NIST Webbook
rinpol	744.00	NIST Webbook
rinpol	746.00	NIST Webbook
rinpol	748.00	NIST Webbook
rinpol	750.00	NIST Webbook
rinpol	752.00	NIST Webbook
rinpol	779.00	NIST Webbook
rinpol	779.20	NIST Webbook
rinpol	749.40	NIST Webbook
rinpol	749.60	NIST Webbook
rinpol	747.00	NIST Webbook
rinpol	747.00	NIST Webbook
rinpol	747.00	NIST Webbook
rinpol	783.10	NIST Webbook
rinpol	738.40	NIST Webbook
rinpol	780.20	NIST Webbook
rinpol	772.00	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	776.00	NIST Webbook
rinpol	779.00	NIST Webbook
rinpol	782.00	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	798.00	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	779.00	NIST Webbook
rinpol	783.00	NIST Webbook
rinpol	788.00	NIST Webbook
rinpol	772.70	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	744.90	NIST Webbook
rinpol	742.04	NIST Webbook
rinpol	749.00	NIST Webbook
rinpol	789.00	NIST Webbook
rinpol	776.00	NIST Webbook
rinpol	783.00	NIST Webbook
rinpol	756.00	NIST Webbook
rinpol	746.00	NIST Webbook

rinpol	751.00	NIST Webbook
rinpol	743.00	NIST Webbook
rinpol	780.00	NIST Webbook
rinpol	736.00	NIST Webbook
rinpol	747.20	NIST Webbook
rinpol	748.10	NIST Webbook
rinpol	749.50	NIST Webbook
rinpol	750.70	NIST Webbook
rinpol	751.60	NIST Webbook
rinpol	752.70	NIST Webbook
rinpol	778.20	NIST Webbook
rinpol	779.60	NIST Webbook
rinpol	781.90	NIST Webbook
rinpol	783.70	NIST Webbook
rinpol	785.20	NIST Webbook
rinpol	786.50	NIST Webbook
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rinpol	779.00	NIST Webbook
rinpol	747.20	NIST Webbook
rinpol	752.70	NIST Webbook
rinpol	785.20	NIST Webbook
rinpol	783.00	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	789.00	NIST Webbook

rinpol	748.00		NIST Webbook
tb	390.70 ± 2.00	K	NIST Webbook
tb	391.30 ± 0.70	K	NIST Webbook
tb	390.35 ± 0.30	K	NIST Webbook
tb	391.30 ± 2.00	K	NIST Webbook
tc	579.97	K	Joback Method
tf	160.25 ± 0.20	K	NIST Webbook
vc	0.422	m3/kmol	Joback Method

Temperature Dependent Properties

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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.26924e+01
Coeff. B	-2.80821e+03
Coeff. C	-5.05480e+01
Temperature range (K), min.	276.93
Temperature range (K), max.	431.02

Sources

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=C15890401&Units=SI
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

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