

Cyclopentane, 1,2,4-trimethyl-, (1«alpha»,2«alpha»,4«beta»)-

Other names:	(1«alpha»,2«alpha»,4«beta»)-1,2,4-trimethylcyclopentane (1Â«alphaÂ»,2Â«alphaÂ»,4Â«betaÂ»)-1,2,4-trimethylcyclopentane 1,2,4-Trimethylcyclopentane, cis, trans 1,cis-2,trans-4-Trimethylcyclopentane 1-cis-2-cis-4-trans-Trimethylcyclopentane 1«alpha»,2«alpha»4«beta»-Trimethylcyclopentane 1Â«alphaÂ»,2Â«alphaÂ»4Â«betaÂ»-Trimethylcyclopentane Cyclopentane, 1,2,4-trimethyl-, cis,trans Cyclopentane, 1,2,4-trimethyl-, cis-1,cis-2,trans-4- cis 1,2-trans-4-trimethylcyclopentane
Inchi:	InChI=1S/C8H16/c1-6-4-7(2)8(3)5-6/h6-8H,4-5H2,1-3H3/t6-,7-,8+
InchiKey:	PNUFYSGVPVMNRN-WHUPJOBBSA-N
Formula:	C8H16
SMILES:	CC1CC(C)C(C)C1
Mol. weight [g/mol]:	112.21
CAS:	4850-28-6

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	774.00		NIST Webbook
rinpol	784.40		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	771.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	780.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	775.40		NIST Webbook
rinpol	778.80		NIST Webbook
rinpol	774.00		NIST Webbook

rinpol	784.40	NIST Webbook
rinpol	769.00	NIST Webbook
rinpol	780.00	NIST Webbook
rinpol	779.00	NIST Webbook
rinpol	772.70	NIST Webbook
rinpol	777.00	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	774.80	NIST Webbook
rinpol	766.00	NIST Webbook
rinpol	769.00	NIST Webbook
rinpol	771.00	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	776.00	NIST Webbook
rinpol	779.00	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	775.40	NIST Webbook
rinpol	740.00	NIST Webbook
rinpol	740.00	NIST Webbook
rinpol	740.00	NIST Webbook
rinpol	737.00	NIST Webbook
rinpol	778.80	NIST Webbook
rinpol	778.80	NIST Webbook
rinpol	773.00	NIST Webbook
rinpol	778.00	NIST Webbook
rinpol	771.00	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	775.00	NIST Webbook
rinpol	777.00	NIST Webbook
rinpol	779.00	NIST Webbook
rinpol	773.60	NIST Webbook
rinpol	771.00	NIST Webbook
rinpol	791.00	NIST Webbook
rinpol	768.00	NIST Webbook
rinpol	774.00	NIST Webbook
rinpol	777.00	NIST Webbook
rinpol	782.00	NIST Webbook
rinpol	783.00	NIST Webbook
rinpol	744.00	NIST Webbook
rinpol	737.00	NIST Webbook
rinpol	776.60	NIST Webbook
rinpol	764.10	NIST Webbook
rinpol	737.00	NIST Webbook
rinpol	768.44	NIST Webbook
rinpol	768.82	NIST Webbook

rmpol	769.00			NIST Webbook
rmpol	784.00			NIST Webbook
rmpol	770.00			NIST Webbook
rmpol	777.00			NIST Webbook
rmpol	776.00			NIST Webbook
rmpol	744.00			NIST Webbook
rmpol	773.00			NIST Webbook
rmpol	774.00			NIST Webbook
rmpol	777.00			NIST Webbook
rmpol	780.00			NIST Webbook
rmpol	782.00			NIST Webbook
tb	390.10 ± 0.30		K	NIST Webbook
tb	390.00 ± 0.30		K	NIST Webbook
tb	389.90 ± 0.60		K	NIST Webbook
tb	390.05 ± 0.30		K	NIST Webbook
tb	389.88 ± 0.20		K	NIST Webbook
tb	389.89 ± 0.30		K	NIST Webbook
tb	389.91 ± 1.00		K	NIST Webbook
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/molxK	388.38	Joback Method
cpg	230.52	J/molxK	420.31	Joback Method
cpg	246.72	J/molxK	452.24	Joback Method
cpg	262.24	J/molxK	484.17	Joback Method
cpg	277.08	J/molxK	516.11	Joback Method
cpg	291.26	J/molxK	548.04	Joback Method
cpg	304.79	J/molxK	579.97	Joback Method
dvisc	0.0010560	Paxs	182.34	Joback Method
dvisc	0.0006962	Paxs	216.68	Joback Method
dvisc	0.0005145	Paxs	251.02	Joback Method
dvisc	0.0004089	Paxs	285.36	Joback Method
dvisc	0.0003414	Paxs	319.70	Joback Method
dvisc	0.0002952	Paxs	354.04	Joback Method
dvisc	0.0002619	Paxs	388.38	Joback Method
hvapt	36.80	kJ/mol	351.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.39348e+01
Coeff. B	-3.21588e+03
Coeff. C	-4.48170e+01
Temperature range (K), min.	280.46
Temperature range (K), max.	417.75

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4850286&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/ci9903071
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
hvapt:	Enthalpy of vaporization at a given temperature
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

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