Cyclopentene, 4,4-dimethyl-

Other names: 4,4-Dimethylcyclopentene
Inchi: InChI=1S/C7H12/c1-7(2)5-3-4-6-7/h3-4H,5-6H2,1-2H3
InchiKey: LKXAUCPURVBMRN-UHFFFAOYSA-N
Formula: C7H12
SMILES: CC1(C)CC=CC1
Mol. weight [g/mol]: 96.17
CAS: 19037-72-0

Physical Properties

Property code	Value	Unit	Source
gf	69.08	kJ/mol	Joback Method
hf	-54.31	kJ/mol	Joback Method
hfus	2.75	kJ/mol	Joback Method
hvap	30.57	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.363		Crippen Method
mcvol	94.330	ml/mol	McGowan Method
pc	3768.41	kPa	Joback Method
rinpol	696.00		NIST Webbook
tb	374.24	K	Joback Method
tc	579.63	K	Joback Method
tf	204.21	K	Joback Method
vc	0.352	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	162.74	J/mol×K	374.24	Joback Method
cpg	177.82	J/mol×K	408.47	Joback Method
cpg	191.74	J/mol×K	442.70	Joback Method
cpg	204.60	J/mol×K	476.93	Joback Method
cpg	216.48	J/mol×K	511.16	Joback Method
cpg	227.50	J/mol×K	545.39	Joback Method
cpg	237.75	J/mol×K	579.63	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.29089e+01
Coeff. B	-2.66979e+03
Coeff. C	-5.08700e+01
Temperature range (K), min.	262.40
Temperature range (K), max.	402.28

Sources

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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol628.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19037720&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices

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