

1,3-Cyclopentadiene, 2-ethyl

Inchi:	InChI=1S/C7H10/c1-2-7-5-3-4-6-7/h3,5-6H,2,4H2,1H3
InchiKey:	CBQAACXHLISDSO-UHFFFAOYSA-N
Formula:	C7H10
SMILES:	CCC1=CCC=C1
Mol. weight [g/mol]:	94.15

Physical Properties

Property code	Value	Unit	Source
gf	102.61	kJ/mol	Joback Method
hf	-2.90	kJ/mol	Joback Method
hfus	8.80	kJ/mol	Joback Method
hvap	32.99	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.283		Crippen Method
mcvol	90.030	ml/mol	McGowan Method
pc	3810.39	kPa	Joback Method
rinpol	724.00		NIST Webbook
rinpol	724.00		NIST Webbook
ripol	930.30		NIST Webbook
ripol	930.30		NIST Webbook
tb	382.81	K	Joback Method
tc	583.26	K	Joback Method
tf	197.83	K	Joback Method
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.27	J/molxK	382.81	Joback Method
cpg	164.20	J/molxK	416.22	Joback Method
cpg	175.48	J/molxK	449.63	Joback Method
cpg	186.13	J/molxK	483.04	Joback Method
cpg	196.18	J/molxK	516.44	Joback Method
cpg	205.66	J/molxK	549.85	Joback Method

cpg	214.59	J/mol×K	583.26	Joback Method
dvisc	0.0022617	Paxs	197.83	Joback Method
dvisc	0.0012370	Paxs	228.66	Joback Method
dvisc	0.0007809	Paxs	259.49	Joback Method
dvisc	0.0005435	Paxs	290.32	Joback Method
dvisc	0.0004056	Paxs	321.15	Joback Method
dvisc	0.0003186	Paxs	351.98	Joback Method
dvisc	0.0002602	Paxs	382.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R40827&Units=SI
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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