Cycloheptene

Other names: (Z)-Cycloheptene
Cycloheptene(Z)
UN 2242
Inchi: InChI=1S/C7H12/c1-2-4-6-7-5-3-1/h1-2H,3-7H2
InchiKey: ZXIJMRYMVAMXQP-UHFFFAOYSA-N
Formula: C7H12
SMILES: C1=CCCCCC1
Mol. weight [g/mol]: 96.17
CAS: 628-92-2

Physical Properties

Property code	Value	Unit	Source
chl	-4428.30	kJ/mol	NIST Webbook
gf	58.08	kJ/mol	Joback Method
hf	-61.53	kJ/mol	Joback Method
hfus	3.77	kJ/mol	Joback Method
hvap	32.38	kJ/mol	Joback Method
ie	9.05 ± 0.15	eV	NIST Webbook
ie	9.12	eV	NIST Webbook
ie	8.87	eV	NIST Webbook
log10ws	-3.18		Aqueous Solubility Prediction Method
log10ws	-3.18		Estimated Solubility Method
logp	2.507		Crippen Method
mcvol	94.330	ml/mol	McGowan Method
pc	3950.57	kPa	Joback Method
rinpol	774.00		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	794.20		NIST Webbook
rinpol	797.00		NIST Webbook
rinpol	808.00		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	794.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	770.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	782.00		NIST Webbook

rinpol	785.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	794.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	770.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	782.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	783.00		NIST Webbook
rinpol	774.00		NIST Webbook
ripol	952.00		NIST Webbook
ripol	917.00		NIST Webbook
ripol	952.00		NIST Webbook
tb	387.21	K	Joback Method
tc	601.57	K	Joback Method
tf	217.00 ± 1.00	K	NIST Webbook
tt	217.55 ± 0.01	K	NIST Webbook
vc	0.340	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.25	J/mol×K	565.84	Joback Method
cpg	189.23	J/mol×K	458.66	Joback Method
cpg	174.29	J/mol×K	422.94	Joback Method
cpg	158.52	J/mol×K	387.21	Joback Method
cpg	203.35	J/mol×K	494.39	Joback Method
cpg	241.07	J/mol×K	601.57	Joback Method
cpg	216.68	J/mol×K	530.12	Joback Method
dvisc	0.0221512	Pa×s	177.51	Joback Method

dvisc	0.0002583	Pa×s	387.21	Joback Method
dvisc	0.0003753	Pa×s	352.26	Joback Method
dvisc	0.0005923	Pa×s	317.31	Joback Method
dvisc	0.0010466	Pa×s	282.36	Joback Method
dvisc	0.0021717	Pa×s	247.41	Joback Method
dvisc	0.0057299	Pa×s	212.46	Joback Method
hfust	0.97	kJ/mol	217.00	NIST Webbook
hvapt	36.70	kJ/mol	281.50	NIST Webbook
hvapt	38.50	kJ/mol	282.00	NIST Webbook
hvapt	36.73	kJ/mol	300.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44295e+01
Coeff. B	-3.42389e+03
Coeff. C	-3.85200e+01
Temperature range (K), min.	280.63
Temperature range (K), max.	414.03

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.67489e+01
Coeff. B	-4.63255e+03
Coeff. C	1.38876e-04
Coeff. D	-2.97789e-10
Temperature range (K), min.	251.15
Temperature range (K), max.	313.15

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C628922&Units=SI

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=615

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=615
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

chl:	Standard liquid enthalpy of combustion
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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume