1,3-Cycloheptadiene

Other names: Cyclohepta-1,3-diene
Inchi: InChI=1S/C7H10/c1-2-4-6-7-5-3-1/h1-4H,5-7H2
InchiKey: GWYPDXLJACEENP-UHFFFAOYSA-N
Formula: C7H10
SMILES: C1=CCCCC=C1
Mol. weight [g/mol]: 94.15
CAS: 4054-38-0

Physical Properties

Property code	Value	Unit	Source
gf	88.04	kJ/mol	Joback Method
hf	-3.75	kJ/mol	Joback Method
hfus	4.99	kJ/mol	Joback Method
hvap	32.67	kJ/mol	Joback Method
ie	8.31	eV	NIST Webbook
ie	8.31 ± 0.03	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
log10ws	-2.35		Crippen Method
logp	2.283		Crippen Method
mcvol	90.030	ml/mol	McGowan Method
pc	4135.61	kPa	Joback Method
rinpol	804.00		NIST Webbook
rinpol	820.30		NIST Webbook
rinpol	811.00		NIST Webbook
rinpol	811.00		NIST Webbook
rinpol	796.00		NIST Webbook
rinpol	820.30		NIST Webbook
rinpol	831.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	804.00		NIST Webbook
ripol	1060.00		NIST Webbook
ripol	1060.00		NIST Webbook
ripol	1060.00		NIST Webbook
tb	393.70	K	NIST Webbook
tc	603.08	K	Joback Method
tf	178.27	K	Joback Method

vc	0.326	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	146.42	J/mol×K	386.37	Joback Method
cpg	160.81	J/mol×K	422.49	Joback Method
cpg	174.38	J/mol×K	458.61	Joback Method
cpg	187.18	J/mol×K	494.73	Joback Method
cpg	199.21	J/mol×K	530.85	Joback Method
cpg	210.51	J/mol×K	566.96	Joback Method
cpg	221.11	J/mol×K	603.08	Joback Method
dvisc	0.0148277	Pa×s	178.27	Joback Method
dvisc	0.0042670	Pa×s	212.95	Joback Method
dvisc	0.0017406	Pa×s	247.64	Joback Method
dvisc	0.0008850	Pa×s	282.32	Joback Method
dvisc	0.0005218	Pa×s	317.00	Joback Method
dvisc	0.0003414	Pa×s	351.69	Joback Method
dvisc	0.0002411	Pa×s	386.37	Joback Method

Sources

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=C4054380&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume