1,4-Cycloheptadiene

Inchi: InChI=1S/C7H10/c1-2-4-6-7-5-3-1/h1-2,5,7H,3-4,6H2
InchiKey: HQGYGGZHZWXFSI-UHFFFAOYSA-N
Formula: C7H10
SMILES: C1=CCCC=CC1
Mol. weight [g/mol]: 94.15
CAS: 7161-35-5

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	8.85 ± 0.03	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	784.00		NIST Webbook
tb	386.37	K	Joback Method
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	210.51	J/mol×K	566.96	Joback Method
cpg	199.21	J/mol×K	530.85	Joback Method
cpg	187.18	J/mol×K	494.73	Joback Method
cpg	174.38	J/mol×K	458.61	Joback Method
cpg	160.81	J/mol×K	422.49	Joback Method
cpg	221.11	J/mol×K	603.08	Joback Method

dvisc	0.0002411	Pa×s	386.37	Joback Method
dvisc	0.0003414	Pa×s	351.69	Joback Method
dvisc	0.0005218	Pa×s	317.00	Joback Method
dvisc	0.0008850	Pa×s	282.32	Joback Method
dvisc	0.0017406	Pa×s	247.64	Joback Method
dvisc	0.0042670	Pa×s	212.95	Joback Method
dvisc	0.0148277	Pa×s	178.27	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=C7161355&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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