

cis-Cycloheptene

Inchi:	InChI=1S/C7H12/c1-2-4-6-7-5-3-1/h1-2H,3-7H2
InchiKey:	ZXIJMRYMVAMXQP-UHFFFAOYSA-N
Formula:	C7H12
SMILES:	C1=CCCCC1
Mol. weight [g/mol]:	96.17
CAS:	45509-99-7

Physical Properties

Property code	Value	Unit	Source
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
log10ws	-2.50		Crippen Method
logp	2.507		Crippen Method
mvol	94.330	ml/mol	McGowan Method
pc	3950.57	kPa	Joback Method
sl	241.00	J/molxK	NIST Webbook
tb	387.21	K	Joback Method
tc	601.57	K	Joback Method
tf	177.51	K	Joback Method
vc	0.340	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.52	J/molxK	387.21	Joback Method
cpg	174.29	J/molxK	422.94	Joback Method
cpg	189.23	J/molxK	458.66	Joback Method
cpg	203.35	J/molxK	494.39	Joback Method
cpg	216.68	J/molxK	530.12	Joback Method
cpg	229.25	J/molxK	565.84	Joback Method
cpg	241.07	J/molxK	601.57	Joback Method
cpl	171.70	J/molxK	298.15	NIST Webbook

dvisc	0.0221512	Paxs	177.51	Joback Method
dvisc	0.0057299	Paxs	212.46	Joback Method
dvisc	0.0021717	Paxs	247.41	Joback Method
dvisc	0.0010466	Paxs	282.36	Joback Method
dvisc	0.0005923	Paxs	317.31	Joback Method
dvisc	0.0003753	Paxs	352.26	Joback Method
dvisc	0.0002583	Paxs	387.21	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=C45509997&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
cp_l:	Liquid phase 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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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