2-Cyclohepten-1-one

Other names: Tropilene
2-Cycloheptenone
cyclohept-2-en-1-one
Inchi: InChI=1S/C7H10O/c8-7-5-3-1-2-4-6-7/h3,5H,1-2,4,6H2
InchiKey: WZCRDVTWUYLPTR-UHFFFAOYSA-N
Formula: C7H10O
SMILES: O=C1C=CCCCC1
Mol. weight [g/mol]: 110.15
CAS: 1121-66-0

Physical Properties

Property code	Value	Unit	Source
gf	-64.51	kJ/mol	Joback Method
hf	-199.23	kJ/mol	Joback Method
hfus	3.28	kJ/mol	Joback Method
hvap	36.62	kJ/mol	Joback Method
ie	9.25	eV	NIST Webbook
log10ws	-1.78		Crippen Method
logp	1.686		Crippen Method
mcvol	95.900	ml/mol	McGowan Method
pc	4130.29	kPa	Joback Method
rinpol	1020.00		NIST Webbook
rinpol	1024.00		NIST Webbook
tb	455.03	K	Joback Method
tc	690.86	K	Joback Method
tf	245.73	K	Joback Method
vc	0.346	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.47	J/mol×K	455.03	Joback Method
cpg	202.54	J/mol×K	494.34	Joback Method
cpg	216.89	J/mol×K	533.64	Joback Method

cpg	230.50	J/mol×K	572.95	Joback Method
cpg	243.38	J/mol×K	612.25	Joback Method
cpg	255.51	J/mol×K	651.56	Joback Method
cpg	266.87	J/mol×K	690.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1121660&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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