1H-Inden-1-one, octahydro-, trans-

Other names: 1-Indanone, hexahydro-, trans-
Octahydro-1H-inden-1-one, (E)-
Inchi: InChI=1S/C9H14O/c10-9-6-5-7-3-1-2-4-8(7)9/h7-8H,1-6H2/t7-,8+/m1/s1
InchiKey: ATKSQUYIHKMKTG-SFYZADRCSA-N
Formula: C9H14O
SMILES: O=C1CCC2CCCCC12
Mol. weight [g/mol]: 138.21
CAS: 16783-22-5

Physical Properties

Property code	Value	Unit	Source
chl	-5193.60	kJ/mol	NIST Webbook
gf	-12.49	kJ/mol	Joback Method
hf	-239.67	kJ/mol	Joback Method
hfus	8.55	kJ/mol	Joback Method
hvap	40.22	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	2.156		Crippen Method
mcvol	117.520	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
tb	499.43	K	Joback Method
tc	734.32	K	Joback Method
tf	284.73	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.47	J/mol×K	499.43	Joback Method
cpg	296.85	J/mol×K	538.58	Joback Method
cpg	315.07	J/mol×K	577.73	Joback Method
cpg	332.18	J/mol×K	616.87	Joback Method
cpg	348.20	J/mol×K	656.02	Joback Method
cpg	363.18	J/mol×K	695.17	Joback Method

cpg	377.14	J/mol×K	734.32	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=C16783225&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume