Ethanone, 1-(2,3-dihydro-1H-inden-5-yl)-

Other names:	Ketone, 5-indanyl methyl
	5-Acetylindan
	5-Acetylindane
	1-Indan-1-ylethanone
Inchi:	InChI=1S/C11H12O/c1-8(12)10-7-6-9-4-2-3-5-11(9)10/h2-5,10H,6-7H2,1H3
InchiKey:	ZDDDIYOBAOJYAZ-UHFFFAOYSA-N
Formula:	C11H12O
SMILES:	CC(=O)C1CCc2ccccc21
Mol. weight [g/mol]:	160.21
CAS:	4228-10-8

Physical Properties

Property code	Value	Unit	Source
gf	76.35	kJ/mol	Joback Method
hf	-85.09	kJ/mol	Joback Method
hfus	17.63	kJ/mol	Joback Method
hvap	49.68	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.305		Crippen Method
mcvol	132.800	ml/mol	McGowan Method
pc	3210.04	kPa	Joback Method
rinpol	1546.00		NIST Webbook
tb	543.35	K	Joback Method
tc	772.49	K	Joback Method
tf	320.54	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.08	J/mol×K	543.35	Joback Method
cpg	373.39	J/mol×K	734.30	Joback Method
cpg	362.02	J/mol×K	696.11	Joback Method
cpg	349.78	J/mol×K	657.92	Joback Method

cpg	336.59	J/mol×K	619.73	Joback Method
cpg	322.38	J/mol×K	581.54	Joback Method
cpg	383.95	J/mol×K	772.49	Joback Method
dvisc	0.0005131	Pa×s	543.35	Joback Method
dvisc	0.0005920	Pa×s	506.21	Joback Method
dvisc	0.0006986	Pa×s	469.08	Joback Method
dvisc	0.0008482	Pa×s	431.94	Joback Method
dvisc	0.0010681	Pa×s	394.81	Joback Method
dvisc	0.0014109	Pa×s	357.68	Joback Method
dvisc	0.0019881	Pa×s	320.54	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	415.00	K	2.00	NIST Webbook

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=C4228108&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume