

(Z)-8-Methyl-1-hydrindanone

Inchi:	InChI=1S/C10H16O/c1-7-3-2-4-8-5-6-9(11)10(7)8/h7-8,10H,2-6H2,1H3/t7-,8-,10-/m1/s1
InchiKey:	NCVVCYYBUJLMQP-NQMVMOMDSA-N
Formula:	C10H16O
SMILES:	CC1CCCC2CCC(=O)C12
Mol. weight [g/mol]:	152.23

Physical Properties

Property code	Value	Unit	Source
gf	-11.78	kJ/mol	Joback Method
hf	-280.65	kJ/mol	Joback Method
hfus	12.21	kJ/mol	Joback Method
hvap	42.13	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.402		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	2950.48	kPa	Joback Method
rinpol	1157.00		NIST Webbook
rinpol	1157.00		NIST Webbook
tb	517.64	K	Joback Method
tc	748.13	K	Joback Method
tf	291.76	K	Joback Method
vc	0.491	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.14	J/mol×K	517.64	Joback Method
cpg	345.76	J/mol×K	556.05	Joback Method
cpg	365.21	J/mol×K	594.47	Joback Method
cpg	383.52	J/mol×K	632.88	Joback Method
cpg	400.72	J/mol×K	671.30	Joback Method
cpg	416.82	J/mol×K	709.71	Joback Method
cpg	431.86	J/mol×K	748.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R626772&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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