

2-Acetyl-1-tetralone

Other names:	2-Acetyltetralone 1(2H)-Naphthalenone, 2-acetyl-3,4-dihydro- 2-acetyl-1,2,3,4-tetrahydronaphthalen-1-one
Inchi:	InChI=1S/C12H12O2/c1-8(13)10-7-6-9-4-2-3-5-11(9)12(10)14/h2-5,10H,6-7H2,1H3
InchiKey:	BSELJBOMYPMBNL-UHFFFAOYSA-N
Formula:	C12H12O2
SMILES:	CC(=O)C1CCc2ccccc2C1=O
Mol. weight [g/mol]:	188.22
CAS:	17216-08-9

Physical Properties

Property code	Value	Unit	Source
gf	-49.92	kJ/mol	Joback Method
hf	-249.59	kJ/mol	Joback Method
hfus	17.63	kJ/mol	Joback Method
hvap	56.32	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.021		Crippen Method
mcvol	148.460	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
rinpol	1518.00		NIST Webbook
tb	638.32	K	Joback Method
tc	884.47	K	Joback Method
tf	396.51	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.70	J/mol×K	638.32	Joback Method
cpg	398.69	J/mol×K	679.35	Joback Method
cpg	413.52	J/mol×K	720.37	Joback Method
cpg	427.23	J/mol×K	761.40	Joback Method
cpg	439.86	J/mol×K	802.42	Joback Method

cpg	451.44	J/mol×K	843.45	Joback Method
cpg	461.99	J/mol×K	884.47	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	411.70	K	0.10	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17216089&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
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

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