

1-(4-Acetylphenyl)-2-methyl-1-propanone

Inchi:	InChI=1S/C12H14O2/c1-8(2)12(14)11-6-4-10(5-7-11)9(3)13/h4-8H,1-3H3
InchiKey:	OKDVJTURSCLUBA-UHFFFAOYSA-N
Formula:	C12H14O2
SMILES:	CC(=O)c1ccc(C(=O)C(C)C)cc1
Mol. weight [g/mol]:	190.24

Physical Properties

Property code	Value	Unit	Source
gf	-107.34	kJ/mol	Joback Method
hf	-296.39	kJ/mol	Joback Method
hfus	20.16	kJ/mol	Joback Method
hvap	58.35	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	2.728		Crippen Method
mcvol	159.320	ml/mol	McGowan Method
pc	2712.67	kPa	Joback Method
rinpol	1551.00		NIST Webbook
rinpol	1551.00		NIST Webbook
tb	612.92	K	Joback Method
tc	834.15	K	Joback Method
tf	348.80	K	Joback Method
vc	0.606	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.15	J/molxK	612.92	Joback Method
cpg	401.36	J/molxK	649.79	Joback Method
cpg	414.65	J/molxK	686.66	Joback Method
cpg	427.07	J/molxK	723.54	Joback Method
cpg	438.63	J/molxK	760.41	Joback Method
cpg	449.38	J/molxK	797.28	Joback Method
cpg	459.34	J/molxK	834.15	Joback Method
dvisc	0.0024558	Paxs	348.80	Joback Method

dvisc	0.0013114	Paxs	392.82	Joback Method
dvisc	0.0007947	Paxs	436.84	Joback Method
dvisc	0.0005278	Paxs	480.86	Joback Method
dvisc	0.0003754	Paxs	524.88	Joback Method
dvisc	0.0002815	Paxs	568.90	Joback Method
dvisc	0.0002200	Paxs	612.92	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R399445&Units=SI

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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