

2-methylcyclopentyl acetate

Inchi:	InChI=1S/C8H14O2/c1-6-4-3-5-8(6)10-7(2)9/h6,8H,3-5H2,1-2H3
InchiKey:	LYFLFZRUQLBWKF-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	CC(=O)OC1CCCC1C
Mol. weight [g/mol]:	142.20

Physical Properties

Property code	Value	Unit	Source
gf	-188.60	kJ/mol	Joback Method
hf	-413.11	kJ/mol	Joback Method
hfus	14.27	kJ/mol	Joback Method
hvap	42.51	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.738		Crippen Method
mcvol	120.160	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
ripol	1160.00		NIST Webbook
tb	469.34	K	Joback Method
tc	672.68	K	Joback Method
tf	258.74	K	Joback Method
vc	0.448	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.34	J/molxK	469.34	Joback Method
cpg	279.80	J/molxK	503.23	Joback Method
cpg	294.56	J/molxK	537.12	Joback Method
cpg	308.62	J/molxK	571.01	Joback Method
cpg	321.99	J/molxK	604.90	Joback Method
cpg	334.68	J/molxK	638.79	Joback Method
cpg	346.70	J/molxK	672.68	Joback Method
dvisc	0.0022929	Paxs	258.74	Joback Method
dvisc	0.0013829	Paxs	293.84	Joback Method

dvisc	0.0009291	Paxs	328.94	Joback Method
dvisc	0.0006740	Paxs	364.04	Joback Method
dvisc	0.0005173	Paxs	399.14	Joback Method
dvisc	0.0004144	Paxs	434.24	Joback Method
dvisc	0.0003432	Paxs	469.34	Joback Method

Sources

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=R322826&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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