Cyclooctanol, acetate

Other names: Cyclooctyl acetate
Inchi: InChI=1S/C10H18O2/c1-9(11)12-10-7-5-3-2-4-6-8-10/h10H,2-8H2,1H3
InchiKey: VBSHAXJPLHCYTH-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: CC(=O)OC1CCCCCCC1
Mol. weight [g/mol]: 170.25
CAS: 772-60-1

Physical Properties

Property code	Value	Unit	Source
gf	-200.35	kJ/mol	Joback Method
hf	-452.53	kJ/mol	Joback Method
hfus	12.08	kJ/mol	Joback Method
hvap	47.78	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.662		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	2838.39	kPa	Joback Method
rinpol	1280.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1279.00		NIST Webbook
ripol	1645.00		NIST Webbook
tb	532.58	K	Joback Method
tc	753.32	K	Joback Method
tf	274.96	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.67	J/mol×K	532.58	Joback Method
cpg	376.63	J/mol×K	569.37	Joback Method

cpg	395.53	J/mol×K	606.16	Joback Method
cpg	413.38	J/mol×K	642.95	Joback Method
cpg	430.17	J/mol×K	679.74	Joback Method
cpg	445.91	J/mol×K	716.53	Joback Method
cpg	460.58	J/mol×K	753.32	Joback Method
dvisc	0.0070282	Pa×s	274.96	Joback Method
dvisc	0.0024190	Pa×s	317.90	Joback Method
dvisc	0.0010731	Pa×s	360.83	Joback Method
dvisc	0.0005659	Pa×s	403.77	Joback Method
dvisc	0.0003375	Pa×s	446.71	Joback Method
dvisc	0.0002204	Pa×s	489.64	Joback Method
dvisc	0.0001541	Pa×s	532.58	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C772601&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

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

vc: Critical Volume