p-Cymene-8-acetate

Other names: p-Cymen-8-ol, acetate
Inchi: InChI=1S/C12H16O2/c1-9-5-7-11(8-6-9)12(3,4)14-10(2)13/h5-8H,1-4H3
InchiKey: LQHSKMQTMCTISH-UHFFFAOYSA-N
Formula: C12H16O2
SMILES: CC(=O)OC(C)(C)c1ccc(C)cc1
Mol. weight [g/mol]: 192.25

Physical Properties

Property code	Value	Unit	Source
gf	-78.14	kJ/mol	Joback Method
hf	-319.50	kJ/mol	Joback Method
hfus	15.86	kJ/mol	Joback Method
hvap	53.10	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.793		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2527.73	kPa	Joback Method
rinpol	1328.00		NIST Webbook
rinpol	1328.00		NIST Webbook
rinpol	1323.00		NIST Webbook
rinpol	1323.00		NIST Webbook
rinpol	1323.00		NIST Webbook
ripol	1680.00		NIST Webbook
tb	578.68	K	Joback Method
tc	798.32	K	Joback Method
tf	338.52	K	Joback Method
vc	0.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.08	J/mol×K	578.68	Joback Method
cpg	412.88	J/mol×K	615.29	Joback Method
cpg	427.67	J/mol×K	651.89	Joback Method

cpg	441.50	J/mol×K	688.50	Joback Method
cpg	454.39	J/mol×K	725.10	Joback Method
cpg	466.41	J/mol×K	761.71	Joback Method
cpg	477.58	J/mol×K	798.32	Joback Method
dvisc	0.0019665	Pa×s	338.52	Joback Method
dvisc	0.0010426	Pa×s	378.55	Joback Method
dvisc	0.0006241	Pa×s	418.57	Joback Method
dvisc	0.0004086	Pa×s	458.60	Joback Method
dvisc	0.0002864	Pa×s	498.63	Joback Method
dvisc	0.0002116	Pa×s	538.65	Joback Method
dvisc	0.0001630	Pa×s	578.68	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=R118266&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
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