24-Methyllophenol acetate

Inchi: InChI=1S/C31H52O2/c1-19(2)20(3)9-10-21(4)25-13-14-27-24-11-12-26-22(5)29(33-23(6)
InchiKey: MPSMORKTRDBZSB-SZUPDOHLSA-N
Formula: C31H52O2
SMILES: CC(=O)OC1CCC2(C)C3CCC4(C)C(CCC4C(C)CCC(C)C(C)C)C3=CCC2C1C
Mol. weight [g/mol]: 456.74

Physical Properties

Property code	Value	Unit	Source
gf	129.91	kJ/mol	Joback Method
hf	-687.98	kJ/mol	Joback Method
hfus	42.82	kJ/mol	Joback Method
hvap	90.52	kJ/mol	Joback Method
log10ws	-8.79		Crippen Method
logp	8.451		Crippen Method
mcvol	407.350	ml/mol	McGowan Method
pc	816.33	kPa	Joback Method
rinpol	3372.00		NIST Webbook
tb	1017.90	K	Joback Method
tc	1250.63	K	Joback Method
tf	564.57	K	Joback Method
vc	1.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1578.55	J/mol×K	1017.90	Joback Method
cpg	1613.43	J/mol×K	1056.69	Joback Method
cpg	1648.98	J/mol×K	1095.48	Joback Method
cpg	1685.55	J/mol×K	1134.26	Joback Method
cpg	1723.50	J/mol×K	1173.05	Joback Method
cpg	1763.17	J/mol×K	1211.84	Joback Method
cpg	1804.91	J/mol×K	1250.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R110559&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
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