24-Ethyllophenol acetate, 24-«alpha»

Inchi: InChI=1S/C32H54O2/c1-9-24(20(2)3)11-10-21(4)26-14-15-28-25-12-13-27-22(5)30(34-2
InchiKey: PGPIOJSFSMAPBR-SHQIXNFRSA-N
Formula: C32H54O2
SMILES: CCC(CCC(C)C1CCC2C3=CCC4C(C)C(OC(C)=O)CCC4(C)C3CCC21C)C(C)C
Mol. weight [g/mol]: 470.77

Physical Properties

Property code	Value	Unit	Source
gf	138.33	kJ/mol	Joback Method
hf	-708.62	kJ/mol	Joback Method
hfus	45.41	kJ/mol	Joback Method
hvap	92.75	kJ/mol	Joback Method
log10ws	-9.21		Crippen Method
logp	8.842		Crippen Method
mcvol	421.440	ml/mol	McGowan Method
pc	773.32	kPa	Joback Method
rinpol	3453.00		NIST Webbook
rinpol	3453.00		NIST Webbook
tb	1040.78	K	Joback Method
tc	1276.11	K	Joback Method
tf	575.84	K	Joback Method
vc	1.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1651.52	J/mol×K	1040.78	Joback Method
cpg	1687.92	J/mol×K	1080.00	Joback Method
cpg	1725.18	J/mol×K	1119.22	Joback Method
cpg	1763.66	J/mol×K	1158.44	Joback Method
cpg	1803.73	J/mol×K	1197.67	Joback Method
cpg	1845.76	J/mol×K	1236.89	Joback Method
cpg	1890.10	J/mol×K	1276.11	Joback Method

Sources

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=R110351&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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