1,4-Dimethylindanyl acetate

Inchi: InChI=1S/C13H16O2/c1-9-5-4-6-12-11(9)7-8-13(12,3)15-10(2)14/h4-6H,7-8H2,1-3H3
InchiKey: PWWBXOPVNRIYAW-UHFFFAOYSA-N
Formula: C13H16O2
SMILES: CC(=O)OC1(C)CCc2c(C)cccc21
Mol. weight [g/mol]: 204.26
CAS: 55669-90-4

Physical Properties

Property code	Value	Unit	Source
gf	-26.93	kJ/mol	Joback Method
hf	-254.82	kJ/mol	Joback Method
hfus	17.31	kJ/mol	Joback Method
hvap	56.05	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.720		Crippen Method
mcvol	166.850	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
rinpol	1658.00		NIST Webbook
rinpol	1658.00		NIST Webbook
tb	616.75	K	Joback Method
tc	844.23	K	Joback Method
tf	401.73	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.61	J/mol×K	616.75	Joback Method
cpg	441.20	J/mol×K	654.66	Joback Method
cpg	455.89	J/mol×K	692.58	Joback Method
cpg	469.82	J/mol×K	730.49	Joback Method
cpg	483.14	J/mol×K	768.40	Joback Method
cpg	496.00	J/mol×K	806.32	Joback Method
cpg	508.55	J/mol×K	844.23	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=C55669904&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