24-Methylene-24-dihydroparkeol acetate

Inchi: InChI=1S/C33H54O2/c1-21(2)22(3)11-12-23(4)25-15-19-33(10)27-13-14-28-30(6,7)29(3
InchiKey: VXHAOJSMBYBPDB-JUXMHOGSSA-N
Formula: C33H54O2
SMILES: C=C(CCC(C)C1CCC2(C)C3CCC4C(C)(CCC(OC(C)=O)C4(C)C)C3=CCC12C)C(C)C
Mol. weight [g/mol]: 482.78

Physical Properties

Property code	Value	Unit	Source
gf	217.50	kJ/mol	Joback Method
hf	-577.86	kJ/mol	Joback Method
hfus	36.34	kJ/mol	Joback Method
hvap	92.47	kJ/mol	Joback Method
log10ws	-9.72		Crippen Method
logp	9.152		Crippen Method
mcvol	431.230	ml/mol	McGowan Method
pc	787.71	kPa	Joback Method
rinpol	3428.00		NIST Webbook
tb	1061.14	K	Joback Method
tc	1302.98	K	Joback Method
tf	634.19	K	Joback Method
vc	1.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1725.61	J/mol×K	1061.14	Joback Method
cpg	1778.99	J/mol×K	1101.45	Joback Method
cpg	1836.51	J/mol×K	1141.75	Joback Method
cpg	1898.81	J/mol×K	1182.06	Joback Method
cpg	1966.55	J/mol×K	1222.37	Joback Method
cpg	2040.37	J/mol×K	1262.67	Joback Method
cpg	2120.91	J/mol×K	1302.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R110504&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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