24-Methyl-24-dihydroparkeol acetate

Inchi: InChI=1S/C33H56O2/c1-21(2)22(3)11-12-23(4)25-15-19-33(10)27-13-14-28-30(6,7)29(3
InchiKey: WDXFTQZWIULFAE-ZLXVBXEDSA-N
Formula: C33H56O2
SMILES: CC(=O)OC1CCC2(C)C3=CCC4(C)C(C(C)CCC(C)C(C)C)CCC4(C)C3CCC2C1(C)C
Mol. weight [g/mol]: 484.80

Physical Properties

Property code	Value	Unit	Source
gf	135.77	kJ/mol	Joback Method
hf	-698.78	kJ/mol	Joback Method
hfus	35.41	kJ/mol	Joback Method
hvap	92.67	kJ/mol	Joback Method
log10ws	-9.63		Crippen Method
logp	9.232		Crippen Method
mcvol	435.530	ml/mol	McGowan Method
pc	770.75	kPa	Joback Method
rinpol	3435.00		NIST Webbook
tb	1064.14	K	Joback Method
tc	1305.57	K	Joback Method
tf	634.91	K	Joback Method
vc	1.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1759.31	J/mol×K	1064.14	Joback Method
cpg	1813.06	J/mol×K	1104.38	Joback Method
cpg	1870.83	J/mol×K	1144.62	Joback Method
cpg	1933.28	J/mol×K	1184.86	Joback Method
cpg	2001.03	J/mol×K	1225.09	Joback Method
cpg	2074.71	J/mol×K	1265.33	Joback Method
cpg	2154.97	J/mol×K	1305.57	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=R110400&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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