((1S,4aR,4bR,10aR)-7-Isopropyl-1,4a-dimethyl-1,2,
acetate

Inchi: InChI=1S/C22H34O2/c1-15(2)17-7-9-19-18(13-17)8-10-20-21(4,14-24-16(3)23)11-6-12-2

InchiKey: JVRVYQYYINXFCM-UHFFFAOYSA-N

Formula: C22H34O2

SMILES: CC(=O)OCC1(C)CCCC2(C)C3CCC(C(C)C)=CC3=CCC12

Mol. weight [g/mol]: 330.50

CAS: 146099-60-7

Physical Properties

Property code	Value	Unit	Source
gf	41.72	kJ/mol	Joback Method
hf	-457.13	kJ/mol	Joback Method
hfus	26.05	kJ/mol	Joback Method
hvap	73.23	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	5.685		Crippen Method
mcvol	287.100	ml/mol	McGowan Method
pc	1411.18	kPa	Joback Method
rinpol	2512.00		NIST Webbook
rinpol	2512.00		NIST Webbook
tb	824.27	K	Joback Method
tc	1052.82	K	Joback Method
tf	501.20	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	948.33	J/mol×K	824.27	Joback Method
cpg	973.27	J/mol×K	862.36	Joback Method
cpg	997.94	J/mol×K	900.45	Joback Method
cpg	1022.61	J/mol×K	938.55	Joback Method
cpg	1047.56	J/mol×K	976.64	Joback Method
cpg	1073.09	J/mol×K	1014.73	Joback Method
cpg	1099.48	J/mol×K	1052.82	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C146099607&Units=SI

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