((1S,4aR,4bS,10aR)-1,4a-Dimethyl-7-(propan-2-yli
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: POURHGVSIKHUNU-UHFFFAOYSA-N

Formula: C22H34O2

SMILES: CC(=O)OCC1(C)CCCC2(C)C3CCC(=C(C)C)C=C3CCC12

Mol. weight [g/mol]: 330.50

CAS: 105255-30-9

Physical Properties

Property code	Value	Unit	Source
gf	60.74	kJ/mol	Joback Method
hf	-431.92	kJ/mol	Joback Method
hfus	27.75	kJ/mol	Joback Method
hvap	73.53	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	5.829		Crippen Method
mcvol	287.100	ml/mol	McGowan Method
pc	1416.50	kPa	Joback Method
rinpol	2578.40		NIST Webbook
rinpol	2578.40		NIST Webbook
tb	827.09	K	Joback Method
tc	1057.88	K	Joback Method
tf	499.32	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	948.79	J/mol×K	827.09	Joback Method
cpg	974.07	J/mol×K	865.56	Joback Method
cpg	999.14	J/mol×K	904.02	Joback Method
cpg	1024.28	J/mol×K	942.49	Joback Method
cpg	1049.80	J/mol×K	980.95	Joback Method
cpg	1076.02	J/mol×K	1019.42	Joback Method
cpg	1103.21	J/mol×K	1057.88	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=C105255309&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