amboryl (acetoxymethyl-isolongifolene) acetate

Inchi: InChI=1S/C18H28O2/c1-11(19)20-10-12-6-7-15(2,3)17-9-13-8-14(17)18(12,17)16(13,4)5

InchiKey: ANPXCNWSCGYEMA-RVXBJCKXSA-N

Formula: C18H28O2

SMILES: CC(=O)OCC1CCC(C)(C)C23CC4CC2C13C4(C)C

Mol. weight [g/mol]: 276.41

Physical Properties

Property code	Value	Unit	Source
gf	76.77	kJ/mol	Joback Method
hf	-362.35	kJ/mol	Joback Method
hfus	17.82	kJ/mol	Joback Method
hvap	58.77	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	4.038		Crippen Method
mcvol	228.480	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rinpol	1782.00		NIST Webbook
rinpol	1782.00		NIST Webbook
tb	697.17	K	Joback Method
tc	921.17	K	Joback Method
tf	522.94	K	Joback Method
vc	0.892	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.23	J/mol×K	697.17	Joback Method
cpg	740.73	J/mol×K	734.50	Joback Method
cpg	762.14	J/mol×K	771.84	Joback Method
cpg	784.00	J/mol×K	809.17	Joback Method
cpg	806.82	J/mol×K	846.50	Joback Method
cpg	831.12	J/mol×K	883.84	Joback Method
cpg	857.44	J/mol×K	921.17	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=R200830&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