Fragranyl acetate

Inchi: InChI=1S/C12H22O2/c1-9(2)11-5-6-12(11,4)7-8-14-10(3)13/h9,11H,5-8H2,1-4H3/t11-,12
InchiKey: WHLCYZCJPXWYQN-VXGBXAGGSA-N
Formula: C12H22O2
SMILES: CC(=O)OCCC1(C)CCC1C(C)C
Mol. weight [g/mol]: 198.30

Physical Properties

Property code	Value	Unit	Source
gf	-150.75	kJ/mol	Joback Method
hf	-479.55	kJ/mol	Joback Method
hfus	16.91	kJ/mol	Joback Method
hvap	49.70	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	3.012		Crippen Method
mcvol	176.520	ml/mol	McGowan Method
pc	2165.35	kPa	Joback Method
rinpol	1335.00		NIST Webbook
tb	556.39	K	Joback Method
tc	753.90	K	Joback Method
tf	316.24	K	Joback Method
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.93	J/mol×K	556.39	Joback Method
cpg	469.84	J/mol×K	589.31	Joback Method
cpg	486.80	J/mol×K	622.23	Joback Method
cpg	502.91	J/mol×K	655.15	Joback Method
cpg	518.25	J/mol×K	688.06	Joback Method
cpg	532.91	J/mol×K	720.98	Joback Method
cpg	546.97	J/mol×K	753.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R603600&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

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