Fragranyl propanoate

Inchi: InChI=1S/C13H22O2/c1-5-12(14)15-9-8-13(4)7-6-11(13)10(2)3/h11H,2,5-9H2,1,3-4H3
InchiKey: JUBMNPQMJVLLON-UHFFFAOYSA-N
Formula: C13H22O2
SMILES: C=C(C)C1CCC1(C)CCOC(=O)CC
Mol. weight [g/mol]: 210.31
CAS: 926039-04-5

Physical Properties

Property code	Value	Unit	Source
gf	-60.60	kJ/mol	Joback Method
hf	-379.27	kJ/mol	Joback Method
hfus	20.43	kJ/mol	Joback Method
hvap	51.72	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	3.322		Crippen Method
mcvol	186.310	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
rinpol	1440.70		NIST Webbook
rinpol	1440.70		NIST Webbook
tb	576.27	K	Joback Method
tc	774.26	K	Joback Method
tf	326.79	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.38	J/mol×K	576.27	Joback Method
cpg	499.13	J/mol×K	609.27	Joback Method
cpg	515.95	J/mol×K	642.27	Joback Method
cpg	531.93	J/mol×K	675.27	Joback Method
cpg	547.17	J/mol×K	708.26	Joback Method
cpg	561.75	J/mol×K	741.26	Joback Method
cpg	575.78	J/mol×K	774.26	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=C926039045&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