2-Butenyl Angelate

Inchi: InChI=1S/C9H14O2/c1-4-6-7-11-9(10)8(3)5-2/h4-6H,7H2,1-3H3/b6-4+,8-5-
InchiKey: KQNAEIIOBYBBAI-NDWVUGOJSA-N
Formula: C9H14O2
SMILES: CC=CCOC(=O)C(C)=CC
Mol. weight [g/mol]: 154.21

Physical Properties

Property code	Value	Unit	Source
gf	-57.13	kJ/mol	Joback Method
hf	-249.24	kJ/mol	Joback Method
hfus	20.95	kJ/mol	Joback Method
hvap	44.78	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.072		Crippen Method
mcvol	136.510	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
rinpol	1086.00		NIST Webbook
tb	489.81	K	Joback Method
tc	683.25	K	Joback Method
tf	239.23	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.78	J/mol×K	489.81	Joback Method
cpg	301.50	J/mol×K	522.05	Joback Method
cpg	313.58	J/mol×K	554.29	Joback Method
cpg	325.06	J/mol×K	586.53	Joback Method
cpg	335.95	J/mol×K	618.77	Joback Method
cpg	346.29	J/mol×K	651.01	Joback Method
cpg	356.10	J/mol×K	683.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R438401&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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