Phenyl ethyl angelate, 2-

Other names: 2-Phenylethyl (Z)-2-methyl-2-butenoate
Inchi: InChI=1S/C13H16O2/c1-3-11(2)13(14)15-10-9-12-7-5-4-6-8-12/h3-8H,9-10H2,1-2H3/b11
InchiKey: KVMWYGAYARXPOL-QDEBKDIKSA-N
Formula: C13H16O2
SMILES: CC=C(C)C(=O)OCCc1ccccc1
Mol. weight [g/mol]: 204.26

Physical Properties

Property code	Value	Unit	Source
gf	8.74	kJ/mol	Joback Method
hf	-212.49	kJ/mol	Joback Method
hfus	25.15	kJ/mol	Joback Method
hvap	56.00	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.738		Crippen Method
mcvol	173.410	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpol	1600.00		NIST Webbook
rinpol	1600.00		NIST Webbook
tb	603.85	K	Joback Method
tc	818.90	K	Joback Method
tf	315.81	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.85	J/mol×K	603.85	Joback Method
cpg	438.37	J/mol×K	639.69	Joback Method
cpg	452.94	J/mol×K	675.53	Joback Method
cpg	466.59	J/mol×K	711.37	Joback Method
cpg	479.36	J/mol×K	747.21	Joback Method
cpg	491.29	J/mol×K	783.06	Joback Method
cpg	502.43	J/mol×K	818.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383581&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