[4-[(E)-2-(4-Acetoxyphenyl)-1-ethyl-but-1-enyl]phe
acetate

Inchi: InChI=1S/C22H24O4/c1-5-21(17-7-11-19(12-8-17)25-15(3)23)22(6-2)18-9-13-20(14-10-1

InchiKey: NFCAKXYIMSRNLP-QURGRASLSA-N

Formula: C22H24O4

SMILES: CCC(=C(CC)c1ccc(OC(C)=O)cc1)c1ccc(OC(C)=O)cc1

Mol. weight [g/mol]: 352.42

CAS: 6533-53-5

Physical Properties

Property code	Value	Unit	Source
gf	-64.80	kJ/mol	Joback Method
hf	-439.25	kJ/mol	Joback Method
hfus	43.20	kJ/mol	Joback Method
hvap	88.87	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	5.268		Crippen Method
mcvol	283.900	ml/mol	McGowan Method
pc	1545.13	kPa	Joback Method
rinpol	2514.00		NIST Webbook
tb	922.58	K	Joback Method
tc	1154.31	K	Joback Method
tf	526.90	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	867.89	J/mol×K	922.58	Joback Method
cpg	882.11	J/mol×K	961.20	Joback Method
cpg	895.06	J/mol×K	999.82	Joback Method
cpg	906.79	J/mol×K	1038.44	Joback Method
cpg	917.39	J/mol×K	1077.06	Joback Method
cpg	926.89	J/mol×K	1115.69	Joback Method
cpg	935.37	J/mol×K	1154.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6533535&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