GERANYL PHENYLACETATE

Other names:	Benzeneacetic acid, 3,7-dimethyl-2,6-octadienyl ester, (E)-
	trans-3,7-Dimethyl-2,6-octadienyl phenylacetate
	Acetic acid, phenyl-, 3,7-dimethyl-2,6-octadienyl ester, (E)-
	Geranyl «alpha»-toluate
	Phenylacetic acid, geranyl ester
Inchi:	InChI=1S/C18H24O2/c1-15(2)8-7-9-16(3)12-13-20-18(19)14-17-10-5-4-6-11-17/h4-6,8,1
InchiKey:	UXAIJXIHZDZMSK-FOWTUZBSSA-N
Formula:	C18H24O2
SMILES:	CC(C)=CCC/C(C)=C/COC(=O)Cc1ccccc1
Mol. weight [g/mol]:	272.39

Physical Properties

Property code	Value	Unit	Source
hf	-315.96	kJ/mol	Cheméo Relay (1.0)
hfus	36.99	kJ/mol	Joback Method
hvap	88.62	kJ/mol	Cheméo Relay (1.0)
ie	8.13	eV	Cheméo Relay (1.0)
logp	4.465		Crippen Method
mcvol	239.560	ml/mol	McGowan Method
tb	604.62	K	Cheméo Relay (1.0)
tf	266.91	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.77	J/mol×K	722.29	Joback Method
cpg	681.03	J/mol×K	757.31	Joback Method
cpg	697.23	J/mol×K	792.33	Joback Method
cpg	712.44	J/mol×K	827.34	Joback Method
cpg	726.73	J/mol×K	862.36	Joback Method
cpg	740.17	J/mol×K	897.38	Joback Method
cpg	752.81	J/mol×K	932.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C102227&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point