Benzoic acid, [(E,E)-3,7,11-trimethyl-2,6,10-dodecatrien-1-yl] ester

Othernames: (2E, 6E)-Farnesyl benzoate
Inchi: InChI=1S/C22H30O2/c1-18(2)10-8-11-19(3)12-9-13-20(4)16-17-24-22(23)21-14-6-5-7-15
InchiKey: IBDUXGXSPANFLU-YEFHWUCQSA-N
Formula: C22H30O2
SMILES: CC(C)=CCCC(C)=CCCC(C)=CCOC(=O)c1ccccc1
Mol. weight [g/mol]: 326.47

Physical Properties

Property code	Value	Unit	Source
gf	227.86	kJ/mol	Joback Method
hf	-183.39	kJ/mol	Joback Method
hfus	46.24	kJ/mol	Joback Method
hvap	76.11	kJ/mol	Joback Method
log10ws	-7.14		Crippen Method
logp	6.263		Crippen Method
mcvol	291.620	ml/mol	McGowan Method
pc	1292.07	kPa	Joback Method
ripol	3132.00		NIST Webbook
ripol	3132.00		NIST Webbook
tb	817.85	K	Joback Method
tc	1028.75	K	Joback Method
tf	379.16	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	867.79	J/mol×K	817.85	Joback Method
cpg	885.72	J/mol×K	853.00	Joback Method
cpg	902.64	J/mol×K	888.15	Joback Method
cpg	918.63	J/mol×K	923.30	Joback Method
cpg	933.79	J/mol×K	958.45	Joback Method
cpg	948.21	J/mol×K	993.60	Joback Method
cpg	961.99	J/mol×K	1028.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U164385&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume