Geranyl benzoate

Other names:	Benzoic acid, geraniol ester
	FEMA No. 2511
	Geraniol benzoate
	trans-3,7-Dimethyl-2,6-octadien-1-yl benzoate
	2,6-Octadien-1-ol, 3,7-dimethyl-, 1-benzoate, (2E)-
	2,6-Octadien-1-ol, 3,7-dimethyl-, benzoate, (2E)-
	2,6-Octadien-1-ol, 3,7-dimethyl, benzoate, (E)-
	Benzoic acid, geranyl ester
Inchi:	InChI=1S/C17H22O2/c1-14(2)8-7-9-15(3)12-13-19-17(18)16-10-5-4-6-11-16/h4-6,8,10-1
InchiKey:	YDVXYTIIPGKIJP-NTCAYCPXSA-N
Formula:	C17H22O2
SMILES:	CC(C)=CCCC(C)=CCOC(=O)c1ccccc1
Mol. weight [g/mol]:	258.36
CAS:	94-48-4

Physical Properties

Property code	Value	Unit	Source
gf	114.09	kJ/mol	Joback Method
hf	-187.62	kJ/mol	Joback Method
hfus	34.40	kJ/mol	Joback Method
hvap	64.94	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.536		Crippen Method
mcvol	225.470	ml/mol	McGowan Method
pc	1796.98	kPa	Joback Method
rinpol	1952.00		NIST Webbook
rinpol	1949.00		NIST Webbook
rinpol	1978.00		NIST Webbook
rinpol	1949.00		NIST Webbook
rinpol	1978.00		NIST Webbook
rinpol	1951.00		NIST Webbook
rinpol	1951.00		NIST Webbook
rinpol	1937.00		NIST Webbook
rinpol	1937.00		NIST Webbook
rinpol	1952.00		NIST Webbook
ripol	2617.00		NIST Webbook
ripol	2617.00		NIST Webbook

tb	699.41	K	Joback Method
tc	912.42	K	Joback Method
tf	341.85	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.89	J/mol×K	699.41	Joback Method
cpg	625.86	J/mol×K	734.91	Joback Method
cpg	641.78	J/mol×K	770.41	Joback Method
cpg	656.70	J/mol×K	805.92	Joback Method
cpg	670.69	J/mol×K	841.42	Joback Method
cpg	683.83	J/mol×K	876.92	Joback Method
cpg	696.17	J/mol×K	912.42	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C94484&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume