

Geranic acid, 2-Phenylethyl ester

Inchi:

InChI=1S/C18H24O2/c1-15(2)8-7-9-16(3)14-18(19)20-13-12-17-10-5-4-6-11-17/h4-6,8,1

InchiKey:

INEYYHSYQXYHAG-JQIJEIRASA-N

Formula:

C18H24O2

SMILES:

CC(C)=CCCC(C)=CC(=O)OCCc1ccccc1

Mol. weight [g/mol]:

272.38

Physical Properties

Property code	Value	Unit	Source
gf	122.51	kJ/mol	Joback Method
hf	-208.26	kJ/mol	Joback Method
hfus	36.99	kJ/mol	Joback Method
hvap	67.17	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	4.465		Crippen Method
mcvol	239.560	ml/mol	McGowan Method
pc	1659.19	kPa	Joback Method
rinpol	2080.80		NIST Webbook
rinpol	2080.80		NIST Webbook
tb	722.29	K	Joback Method
tc	932.40	K	Joback Method
tf	353.12	K	Joback Method
vc	0.921	m3/kmol	Joback Method

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U413780&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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