

Benzenepropanoic acid, 3,7-dimethylocta-2,6-dienyl ester

Other names:	geranyl 3-phenylpropanoate
Inchi:	InChI=1S/C19H26O2/c1-16(2)8-7-9-17(3)14-15-21-19(20)13-12-18-10-5-4-6-11-18/h4-6,
InchiKey:	RNXGADQWNZYSFZ-SAPNQHFASA-N
Formula:	C19H26O2
SMILES:	CC(C)=CCCC(C)=CCOC(=O)CCc1ccccc1
Mol. weight [g/mol]:	286.41
CAS:	74339-36-9

Physical Properties

Property code	Value	Unit	Source
gf	130.93	kJ/mol	Joback Method
hf	-228.90	kJ/mol	Joback Method
hfus	39.58	kJ/mol	Joback Method
hvap	69.40	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.855		Crippen Method
mcvol	253.650	ml/mol	McGowan Method
pc	1536.66	kPa	Joback Method
rinpol	2125.00		NIST Webbook
rinpol	2125.00		NIST Webbook
ripol	2740.00		NIST Webbook
ripol	2765.00		NIST Webbook
tb	745.17	K	Joback Method
tc	952.83	K	Joback Method
tf	364.39	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.77	J/molxK	745.17	Joback Method
cpg	737.28	J/molxK	779.78	Joback Method
cpg	753.73	J/molxK	814.39	Joback Method
cpg	769.20	J/molxK	849.00	Joback Method

cpg	783.75	J/mol×K	883.61	Joback Method
cpg	797.45	J/mol×K	918.22	Joback Method
cpg	810.37	J/mol×K	952.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74339369&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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