dehydrogeranyl 3-phenylpropanoate

Inchi: InChI=1S/C19H24O2/c1-16(2)8-7-9-17(3)14-15-21-19(20)13-12-18-10-5-4-6-11-18/h4-11
InchiKey: LDBNQBHQAIZJJT-KTQXPTQNSA-N
Formula: C19H24O2
SMILES: CC(C)=CC=CC(C)=CCOC(=O)CCc1ccccc1
Mol. weight [g/mol]: 284.39

Physical Properties

Property code	Value	Unit	Source
gf	211.15	kJ/mol	Joback Method
hf	-111.68	kJ/mol	Joback Method
hfus	39.78	kJ/mol	Joback Method
hvap	69.35	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	4.631		Crippen Method
mcvol	249.350	ml/mol	McGowan Method
pc	1601.28	kPa	Joback Method
rinpol	2060.00		NIST Webbook
rinpol	2060.00		NIST Webbook
rinpol	2125.00		NIST Webbook
ripol	2790.00		NIST Webbook
tb	749.33	K	Joback Method
tc	963.84	K	Joback Method
tf	359.31	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.62	J/mol×K	749.33	Joback Method
cpg	712.67	J/mol×K	785.08	Joback Method
cpg	728.67	J/mol×K	820.83	Joback Method
cpg	743.72	J/mol×K	856.58	Joback Method
cpg	757.90	J/mol×K	892.34	Joback Method
cpg	771.30	J/mol×K	928.09	Joback Method

cpg	784.01	J/mol×K	963.84	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=R259644&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