Succinic acid, 3-methylbut-2-yl geranyl ester

Inchi: InChI=1S/C19H32O4/c1-14(2)8-7-9-16(5)12-13-22-18(20)10-11-19(21)23-17(6)15(3)4/h8
InchiKey: ZWQLBJVZPXVSNQ-FOWTUZBSSA-N
Formula: C19H32O4
SMILES: CC(C)=CCCC(C)=CCOC(=O)CCC(=O)OC(C)C(C)C
Mol. weight [g/mol]: 324.45

Physical Properties

Property code	Value	Unit	Source
gf	-220.28	kJ/mol	Joback Method
hf	-720.79	kJ/mol	Joback Method
hfus	41.28	kJ/mol	Joback Method
hvap	75.50	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.590		Crippen Method
mcvol	284.850	ml/mol	McGowan Method
pc	1257.48	kPa	Joback Method
rinpol	2139.00		NIST Webbook
rinpol	2139.00		NIST Webbook
tb	793.90	K	Joback Method
tc	987.06	K	Joback Method
tf	380.13	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	859.34	J/mol×K	793.90	Joback Method
cpg	876.61	J/mol×K	826.09	Joback Method
cpg	892.91	J/mol×K	858.29	Joback Method
cpg	908.26	J/mol×K	890.48	Joback Method
cpg	922.72	J/mol×K	922.67	Joback Method
cpg	936.31	J/mol×K	954.87	Joback Method
cpg	949.06	J/mol×K	987.06	Joback Method

Sources

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=U391210&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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