Succinic acid, 2-ethylhexyl geranyl ester

Inchi: InChI=1S/C22H38O4/c1-6-8-12-20(7-2)17-26-22(24)14-13-21(23)25-16-15-19(5)11-9-10
InchiKey: JRYFMNHVDFYNJA-XDJHFCHBSA-N
Formula: C22H38O4
SMILES: CCCCC(CC)COC(=O)CCC(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 366.53

Physical Properties

Property code	Value	Unit	Source
gf	-192.58	kJ/mol	Joback Method
hf	-777.43	kJ/mol	Joback Method
hfus	52.57	kJ/mol	Joback Method
hvap	82.57	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	5.762		Crippen Method
mcvol	327.120	ml/mol	McGowan Method
pc	1029.92	kPa	Joback Method
rinpol	2458.00		NIST Webbook
rinpol	2458.00		NIST Webbook
tb	862.98	K	Joback Method
tc	1059.49	K	Joback Method
tf	428.94	K	Joback Method
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1039.11	J/mol×K	862.98	Joback Method
cpg	1057.26	J/mol×K	895.73	Joback Method
cpg	1074.35	J/mol×K	928.48	Joback Method
cpg	1090.43	J/mol×K	961.24	Joback Method
cpg	1105.53	J/mol×K	993.99	Joback Method
cpg	1119.71	J/mol×K	1026.74	Joback Method
cpg	1133.01	J/mol×K	1059.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391214&Units=SI
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

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

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