

Sebacic acid, geranyl isohexyl ester

Inchi:	InChI=1S/C26H46O4/c1-22(2)14-12-16-24(5)19-21-30-26(28)18-11-9-7-6-8-10-17-25(27)
InchiKey:	SJAHAIHZFVSTDM-LYBHJNIIJSA-N
Formula:	C26H46O4
SMILES:	CC(C)=CCCC(C)=CCOC(=O)CCCCCCCCC(=O)OCCCC(C)C
Mol. weight [g/mol]:	422.64

Physical Properties

Property code	Value	Unit	Source
gf	-158.90	kJ/mol	Joback Method
hf	-859.99	kJ/mol	Joback Method
hfus	62.93	kJ/mol	Joback Method
hvap	91.47	kJ/mol	Joback Method
log10ws	-7.90		Crippen Method
logp	7.322		Crippen Method
mcvol	383.480	ml/mol	McGowan Method
pc	816.33	kPa	Joback Method
rinsol	2908.00		NIST Webbook
tb	954.50	K	Joback Method
tc	1169.68	K	Joback Method
tf	474.02	K	Joback Method
vc	1.496	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1289.42	J/mol×K	954.50	Joback Method
cpg	1309.42	J/mol×K	990.36	Joback Method
cpg	1328.11	J/mol×K	1026.23	Joback Method
cpg	1345.56	J/mol×K	1062.09	Joback Method
cpg	1361.85	J/mol×K	1097.96	Joback Method
cpg	1377.05	J/mol×K	1133.82	Joback Method
cpg	1391.25	J/mol×K	1169.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356101&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mccvol:	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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