

Sebacic acid, digeranyl ester

Inchi:	InChI=1S/C30H50O4/c1-25(2)15-13-17-27(5)21-23-33-29(31)19-11-9-7-8-10-12-20-30(3)
InchiKey:	ZIACLYHJEXVRCW-GPAWKIAZSA-N
Formula:	C30H50O4
SMILES:	<chem>CC(C)=CCCC(C)=CCOC(=O)CCCCCCCCC(=O)OCC=C(C)CCC=C(C)C</chem>
Mol. weight [g/mol]:	474.72

Physical Properties

Property code	Value	Unit	Source
gf	20.56	kJ/mol	Joback Method
hf	-722.41	kJ/mol	Joback Method
hfus	74.60	kJ/mol	Joback Method
hvap	100.84	kJ/mol	Joback Method
log10ws	-9.52		Crippen Method
logp	8.579		Crippen Method
mcvol	431.240	ml/mol	McGowan Method
pc	700.61	kPa	Joback Method
rinsol	3345.00		NIST Webbook
tb	1054.54	K	Joback Method
tc	1299.93	K	Joback Method
tf	496.02	K	Joback Method
vc	1.688	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1490.66	J/mol×K	1054.54	Joback Method
cpg	1513.13	J/mol×K	1095.44	Joback Method
cpg	1534.50	J/mol×K	1136.34	Joback Method
cpg	1554.93	J/mol×K	1177.24	Joback Method
cpg	1574.60	J/mol×K	1218.14	Joback Method
cpg	1593.68	J/mol×K	1259.03	Joback Method
cpg	1612.34	J/mol×K	1299.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356108&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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