

Sebacic acid, decyl geranyl ester

Inchi:	InChI=1S/C30H54O4/c1-5-6-7-8-9-12-15-18-25-33-29(31)22-16-13-10-11-14-17-23-30(3
InchiKey:	BPRBASGIFRBDPM-ZZIIHQDSA-N
Formula:	C30H54O4
SMILES:	CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]:	478.75

Physical Properties

Property code	Value	Unit	Source
gf	-122.78	kJ/mol	Joback Method
hf	-937.27	kJ/mol	Joback Method
hfus	76.81	kJ/mol	Joback Method
hvap	100.76	kJ/mol	Joback Method
log10ws	-9.81		Crippen Method
logp	9.027		Crippen Method
mvol	439.840	ml/mol	McGowan Method
pc	660.17	kPa	Joback Method
rinpol	3355.00		NIST Webbook
rinpol	3355.00		NIST Webbook
tb	1046.46	K	Joback Method
tc	1300.67	K	Joback Method
tf	534.10	K	Joback Method
vc	1.726	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1547.94	J/mol×K	1046.46	Joback Method
cpg	1571.07	J/mol×K	1088.83	Joback Method
cpg	1592.46	J/mol×K	1131.20	Joback Method
cpg	1612.24	J/mol×K	1173.57	Joback Method
cpg	1630.56	J/mol×K	1215.94	Joback Method
cpg	1647.57	J/mol×K	1258.31	Joback Method
cpg	1663.40	J/mol×K	1300.67	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=U356106&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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