

Geranyl palmitoleate

Inchi: InChI=1S/C26H46O2/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-21-26(27)28-23-22-25(4)20
InchiKey: LSHLMRRKUOWTIW-PYHWRHASSA-N
Formula: C26H46O2
SMILES: CCCCCC=CCCCCCCC(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 390.64

Physical Properties

Property code	Value	Unit	Source
gf	157.68	kJ/mol	Joback Method
hf	-492.69	kJ/mol	Joback Method
hfus	63.87	kJ/mol	Joback Method
hvap	82.66	kJ/mol	Joback Method
log10ws	-9.13		Crippen Method
logp	8.480		Crippen Method
mvol	371.740	ml/mol	McGowan Method
pc	815.39	kPa	Joback Method
rinpol	2730.00		NIST Webbook
rinpol	2730.00		NIST Webbook
tb	882.81	K	Joback Method
tc	1081.02	K	Joback Method
tf	411.78	K	Joback Method
vc	1.458	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1205.79	J/mol×K	882.81	Joback Method
cpg	1226.82	J/mol×K	915.85	Joback Method
cpg	1246.82	J/mol×K	948.88	Joback Method
cpg	1265.87	J/mol×K	981.92	Joback Method
cpg	1284.05	J/mol×K	1014.95	Joback Method
cpg	1301.45	J/mol×K	1047.99	Joback Method
cpg	1318.15	J/mol×K	1081.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U414433&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
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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