(2E,6E)-Methyl 10,11-dihydroxy-3,7,11-trimethyldodeca-2,6-dieno

Inchi: InChI=1S/C16H28O4/c1-12(9-10-14(17)16(3,4)19)7-6-8-13(2)11-15(18)20-5/h7,11,14,17

InchiKey: MBJDYYPZJXVUHJ-ZPLWXOMKSA-N

Formula: C16H28O4

SMILES: COC(=O)C=C(C)CCC=C(C)CCC(O)C(C)(C)O

Mol. weight [g/mol]: 284.39

CAS: 36999-94-7

Physical Properties

Property code	Value	Unit	Source
gf	-279.98	kJ/mol	Joback Method
hf	-722.00	kJ/mol	Joback Method
hfus	35.01	kJ/mol	Joback Method
hvap	92.12	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	2.744		Crippen Method
mcvol	246.880	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpol	1788.10		NIST Webbook
rinpol	1788.10		NIST Webbook
tb	830.54	K	Joback Method
tc	1021.48	K	Joback Method
tf	413.22	K	Joback Method
vc	0.939	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.36	J/mol×K	830.54	Joback Method
cpg	778.82	J/mol×K	862.36	Joback Method
cpg	791.60	J/mol×K	894.19	Joback Method
cpg	803.76	J/mol×K	926.01	Joback Method
cpg	815.35	J/mol×K	957.84	Joback Method
cpg	826.44	J/mol×K	989.66	Joback Method
cpg	837.08	J/mol×K	1021.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36999947&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

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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