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

Inchi: InChI=1S/C16H26O3/c1-12(2)15(17)10-9-13(3)7-6-8-14(4)11-16(18)19-5/h7,11,15,17H,1
InchiKey: XCDIUVKHQADBDV-FYCHQBGDSA-N
Formula: C16H26O3
SMILES: C=C(C)C(O)CCC(C)=CCCC(C)=CC(=O)OC
Mol. weight [g/mol]: 266.38

Physical Properties

Property code	Value	Unit	Source
gf	-66.71	kJ/mol	Joback Method
hf	-445.38	kJ/mol	Joback Method
hfus	35.74	kJ/mol	Joback Method
hvap	76.14	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.549		Crippen Method
mcvol	236.710	ml/mol	McGowan Method
pc	1670.06	kPa	Joback Method
rinpol	2017.00		NIST Webbook
rinpol	2017.00		NIST Webbook
tb	738.15	K	Joback Method
tc	923.71	K	Joback Method
tf	334.26	K	Joback Method
vc	0.912	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.87	J/mol×K	738.15	Joback Method
cpg	691.60	J/mol×K	769.08	Joback Method
cpg	705.59	J/mol×K	800.00	Joback Method
cpg	718.88	J/mol×K	830.93	Joback Method
cpg	731.51	J/mol×K	861.85	Joback Method
cpg	743.52	J/mol×K	892.78	Joback Method
cpg	754.97	J/mol×K	923.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R341456&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