

(E)-1-(4-Hydroxy-3-methoxyphenyl)dodec-3-en-5-ol

Inchi:	InChI=1S/C19H28O3/c1-3-4-5-6-7-11-17(20)12-9-8-10-16-13-14-18(21)19(15-16)22-2/h
InchiKey:	ZZSJGFXDTNAIDC-FMIVXFBMSA-N
Formula:	C19H28O3
SMILES:	CCCCCCCC(=O)C=CCCc1ccc(O)c(OC)c1
Mol. weight [g/mol]:	304.42

Physical Properties

Property code	Value	Unit	Source
gf	-96.44	kJ/mol	Joback Method
hf	-515.32	kJ/mol	Joback Method
hfus	47.39	kJ/mol	Joback Method
hvap	82.95	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.819		Crippen Method
mcvol	263.820	ml/mol	McGowan Method
pc	1627.22	kPa	Joback Method
rinsol	2444.60		NIST Webbook
tb	826.85	K	Joback Method
tc	1034.02	K	Joback Method
tf	521.63	K	Joback Method
vc	0.962	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.94	J/molxK	826.85	Joback Method
cpg	819.97	J/molxK	861.38	Joback Method
cpg	835.23	J/molxK	895.91	Joback Method
cpg	849.79	J/molxK	930.44	Joback Method
cpg	863.74	J/molxK	964.96	Joback Method
cpg	877.15	J/molxK	999.49	Joback Method
cpg	890.12	J/molxK	1034.02	Joback Method
dvisc	0.0001298	Paxs	521.63	Joback Method
dvisc	0.0000560	Paxs	572.50	Joback Method

dvisc	0.0000277	Paxs	623.37	Joback Method
dvisc	0.0000152	Paxs	674.24	Joback Method
dvisc	0.0000091	Paxs	725.11	Joback Method
dvisc	0.0000058	Paxs	775.98	Joback Method
dvisc	0.0000039	Paxs	826.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U412840&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
dvisc:	Dynamic viscosity
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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