

(E)-1-(4-Hydroxy-3-methoxyphenyl)hexadec-4-en-

Inchi:	InChI=1S/C23H36O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-21(24)17-15-20-16-18-22(25)23(
InchiKey:	WCQFXNQALHURHS-BUHFOSPRSA-N
Formula:	C23H36O3
SMILES:	CCCCCCCCCCCC=CC(=O)CCc1ccc(O)c(OC)c1
Mol. weight [g/mol]:	360.53
CAS:	104264-52-0

Physical Properties

Property code	Value	Unit	Source
gf	-62.76	kJ/mol	Joback Method
hf	-597.88	kJ/mol	Joback Method
hfus	57.75	kJ/mol	Joback Method
hvap	91.86	kJ/mol	Joback Method
log10ws	-6.94		Crippen Method
logp	6.380		Crippen Method
mcvol	320.180	ml/mol	McGowan Method
pc	1219.99	kPa	Joback Method
rinpol	2937.70		NIST Webbook
rinpol	2937.70		NIST Webbook
tb	918.37	K	Joback Method
tc	1128.58	K	Joback Method
tf	566.71	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1043.46	J/molxK	918.37	Joback Method
cpg	1061.25	J/molxK	953.41	Joback Method
cpg	1078.25	J/molxK	988.44	Joback Method
cpg	1094.58	J/molxK	1023.48	Joback Method
cpg	1110.34	J/molxK	1058.51	Joback Method
cpg	1125.60	J/molxK	1093.55	Joback Method
cpg	1140.49	J/molxK	1128.58	Joback Method

dvisc	0.0000635	Paxs	566.71	Joback Method
dvisc	0.0000264	Paxs	625.32	Joback Method
dvisc	0.0000127	Paxs	683.93	Joback Method
dvisc	0.0000069	Paxs	742.54	Joback Method
dvisc	0.0000041	Paxs	801.15	Joback Method
dvisc	0.0000026	Paxs	859.76	Joback Method
dvisc	0.0000017	Paxs	918.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104264520&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
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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