(E)-1-(4-Hydroxy-3-methoxyphenyl)tetradec-3-en-5

Inchi: InChI=1S/C21H32O3/c1-3-4-5-6-7-8-9-13-19(22)14-11-10-12-18-15-16-20(23)21(17-18)2
InchiKey: ICGMHNGYISGRQK-SDNWHVSQSA-N
Formula: C21H32O3
SMILES: CCCCCCCCCC(=O)C=CCCc1ccc(O)c(OC)c1
Mol. weight [g/mol]: 332.48
CAS: 1278586-98-3

Physical Properties

Property code	Value	Unit	Source
gf	-79.60	kJ/mol	Joback Method
hf	-556.60	kJ/mol	Joback Method
hfus	52.57	kJ/mol	Joback Method
hvap	87.41	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	5.599		Crippen Method
mcvol	292.000	ml/mol	McGowan Method
pc	1401.69	kPa	Joback Method
rinpol	2652.80		NIST Webbook
rinpol	2652.80		NIST Webbook
tb	872.61	K	Joback Method
tc	1079.80	K	Joback Method
tf	544.17	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	921.96	J/mol×K	872.61	Joback Method
cpg	938.81	J/mol×K	907.14	Joback Method
cpg	954.89	J/mol×K	941.67	Joback Method
cpg	970.28	J/mol×K	976.21	Joback Method
cpg	985.07	J/mol×K	1010.74	Joback Method
cpg	999.35	J/mol×K	1045.27	Joback Method
cpg	1013.21	J/mol×K	1079.80	Joback Method

dvisc	0.0000909	Pa×s	544.17	Joback Method
dvisc	0.0000384	Pa×s	598.91	Joback Method
dvisc	0.0000188	Pa×s	653.65	Joback Method
dvisc	0.0000102	Pa×s	708.39	Joback Method
dvisc	0.0000061	Pa×s	763.13	Joback Method
dvisc	0.0000039	Pa×s	817.87	Joback Method
dvisc	0.0000026	Pa×s	872.61	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1278586983&Units=SI

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