1-(4-hydroxy-3-methoxyphenyl)tetradec-1-ene-3,5

Inchi: InChI=1S/C21H30O4/c1-3-4-5-6-7-8-9-10-18(22)16-19(23)13-11-17-12-14-20(24)21(15-1
InchiKey: QJDGTTCAEQPSJA-ACCUITESSA-N
Formula: C21H30O4
SMILES: CCCCCCCCCC(=O)CC(=O)C=Cc1ccc(O)c(OC)c1
Mol. weight [g/mol]: 346.46
CAS: 136826-50-1

Physical Properties

Property code	Value	Unit	Source
gf	-208.52	kJ/mol	Joback Method
hf	-669.18	kJ/mol	Joback Method
hfus	54.17	kJ/mol	Joback Method
hvap	94.15	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	5.083		Crippen Method
mcvol	293.570	ml/mol	McGowan Method
pc	1470.23	kPa	Joback Method
rinpol	3028.10		NIST Webbook
rinpol	3028.10		NIST Webbook
tb	926.48	K	Joback Method
tc	1141.95	K	Joback Method
tf	594.10	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	938.18	J/mol×K	926.48	Joback Method
cpg	953.87	J/mol×K	962.39	Joback Method
cpg	968.86	J/mol×K	998.30	Joback Method
cpg	983.23	J/mol×K	1034.21	Joback Method
cpg	997.10	J/mol×K	1070.13	Joback Method
cpg	1010.55	J/mol×K	1106.04	Joback Method
cpg	1023.68	J/mol×K	1141.95	Joback Method

dvisc	0.0000559	Pa×s	594.10	Joback Method
dvisc	0.0000258	Pa×s	649.50	Joback Method
dvisc	0.0000135	Pa×s	704.89	Joback Method
dvisc	0.0000077	Pa×s	760.29	Joback Method
dvisc	0.0000048	Pa×s	815.69	Joback Method
dvisc	0.0000031	Pa×s	871.08	Joback Method
dvisc	0.0000022	Pa×s	926.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C136826501&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
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