(E)-1,7-bis(4-Hydroxy-3-methoxyphenyl)hept-4-en

Inchi: InChI=1S/C21H24O5/c1-25-20-13-15(8-11-18(20)23)5-3-4-6-17(22)10-7-16-9-12-19(24)2
InchiKey: FWDXZNKYDTXGOT-GQCTYLIASA-N
Formula: C21H24O5
SMILES: COc1cc(CCC=CC(=O)CCc2ccc(O)c(OC)c2)ccc1O
Mol. weight [g/mol]: 356.41
CAS: 128700-97-0

Physical Properties

Property code	Value	Unit	Source
gf	-236.44	kJ/mol	Joback Method
hf	-641.07	kJ/mol	Joback Method
hfus	53.19	kJ/mol	Joback Method
hvap	105.77	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.806		Crippen Method
mcvol	279.980	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
rinpol	3158.80		NIST Webbook
rinpol	3158.80		NIST Webbook
tb	1007.31	K	Joback Method
tc	1247.99	K	Joback Method
tf	717.06	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	902.77	J/mol×K	1007.31	Joback Method
cpg	918.49	J/mol×K	1047.42	Joback Method
cpg	934.08	J/mol×K	1087.54	Joback Method
cpg	949.73	J/mol×K	1127.65	Joback Method
cpg	965.60	J/mol×K	1167.77	Joback Method
cpg	981.86	J/mol×K	1207.88	Joback Method
cpg	998.67	J/mol×K	1247.99	Joback Method

dvisc	0.0000011	Pa×s	717.06	Joback Method
dvisc	0.0000005	Pa×s	765.43	Joback Method
dvisc	0.0000003	Pa×s	813.81	Joback Method
dvisc	0.0000002	Pa×s	862.18	Joback Method
dvisc	0.0000001	Pa×s	910.56	Joback Method
dvisc	7.1186132e-08	Pa×s	958.93	Joback Method
dvisc	4.8301378e-08	Pa×s	1007.31	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=C128700970&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