

(Z)-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-XQRVVYSFSA-N
Formula:	C21H24O5
SMILES:	COc1cc(CCC=CC(=O)CCc2ccc(O)c(OC)c2)ccc1O
Mol. weight [g/mol]:	356.41
CAS:	81569-02-0

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	3103.30		NIST Webbook
rinpol	3103.30		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/molxK	1007.31	Joback Method
cpg	918.49	J/molxK	1047.42	Joback Method
cpg	934.08	J/molxK	1087.54	Joback Method
cpg	949.73	J/molxK	1127.65	Joback Method
cpg	965.60	J/molxK	1167.77	Joback Method
cpg	981.86	J/molxK	1207.88	Joback Method
cpg	998.67	J/molxK	1247.99	Joback Method

dvisc	0.0000011	Paxs	717.06	Joback Method
dvisc	0.0000005	Paxs	765.43	Joback Method
dvisc	0.0000003	Paxs	813.81	Joback Method
dvisc	0.0000002	Paxs	862.18	Joback Method
dvisc	0.0000001	Paxs	910.56	Joback Method
dvisc	7.1186132e-08	Paxs	958.93	Joback Method
dvisc	4.8301378e-08	Paxs	1007.31	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C81569020&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
mvol:	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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