2-dehydro-O -demethylangolensin [1 -(2',4"-dihydroxyphenyl)-2-(4"-hydroxyphenyl)-pro 1-one]

Inchi: InChI=1S/C15H12O4/c1-9(10-2-4-11(16)5-3-10)15(19)13-7-6-12(17)8-14(13)18/h2-8,16-

InchiKey: MPNKZWIUITZJCR-UHFFFAOYSA-N

Formula: C15H12O4

SMILES: C=C(C(=O)c1ccc(O)cc1O)c1ccc(O)cc1

Mol. weight [g/mol]: 256.25

Physical Properties

Property code	Value	Unit	Source
gf	-213.25	kJ/mol	Joback Method
hf	-408.74	kJ/mol	Joback Method
hfus	39.05	kJ/mol	Joback Method
hvap	98.73	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.700		Crippen Method
mcvol	189.570	ml/mol	McGowan Method
pc	4829.24	kPa	Joback Method
rinpol	2592.00		NIST Webbook
tb	888.25	K	Joback Method
tc	1156.36	K	Joback Method
tf	681.02	K	Joback Method
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.32	J/mol×K	888.25	Joback Method
cpg	563.82	J/mol×K	932.94	Joback Method
cpg	576.83	J/mol×K	977.62	Joback Method
cpg	590.68	J/mol×K	1022.31	Joback Method
cpg	605.71	J/mol×K	1066.99	Joback Method
cpg	622.25	J/mol×K	1111.68	Joback Method
cpg	640.64	J/mol×K	1156.36	Joback Method

Sources

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=R261424&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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