2H-1-Benzopyran-3-ol, 2-(3,4-dimethoxyphenyl)-3,4-dihydro-5,7-dimethox (2R-trans)-

Other names: Catechin, tetramethyl
Inchi: InChI=1S/C19H22O6/c1-21-12-8-16(23-3)13-10-14(20)19(25-17(13)9-12)11-5-6-15(22-2
InchiKey: GKPNPQODFXMCGO-KUHUBIRLSA-N
Formula: C19H22O6
SMILES: COc1cc(OC)c2c(c1)OC(c1ccc(OC)c(OC)c1)C(O)C2
Mol. weight [g/mol]: 346.37
CAS: 51079-25-5

Physical Properties

Property code	Value	Unit	Source
gf	-316.23	kJ/mol	Joback Method
hf	-786.59	kJ/mol	Joback Method
hfus	45.03	kJ/mol	Joback Method
hvap	96.35	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	2.758		Crippen Method
mcvol	255.410	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	2959.00		NIST Webbook
rinpol	2959.00		NIST Webbook
tb	927.53	K	Joback Method
tc	1149.49	K	Joback Method
tf	605.82	K	Joback Method
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	824.28	J/mol×K	927.53	Joback Method
cpg	836.91	J/mol×K	964.52	Joback Method
cpg	848.10	J/mol×K	1001.52	Joback Method
cpg	857.82	J/mol×K	1038.51	Joback Method
cpg	866.07	J/mol×K	1075.50	Joback Method
cpg	872.84	J/mol×K	1112.50	Joback Method

cpg	878.11	J/mol×K	1149.49	Joback Method
dvisc	0.0001307	Pa×s	605.82	Joback Method
dvisc	0.0000785	Pa×s	659.44	Joback Method
dvisc	0.0000509	Pa×s	713.06	Joback Method
dvisc	0.0000351	Pa×s	766.68	Joback Method
dvisc	0.0000254	Pa×s	820.29	Joback Method
dvisc	0.0000191	Pa×s	873.91	Joback Method
dvisc	0.0000149	Pa×s	927.53	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51079255&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

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

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