2H-1-Benzopyran, 3,4-dihydro-4-(4-hydroxyphenyl)-2,2,4-trimethyl-

Other names: p-(2,2,4-Trimethyl-4-chromanyl)phenol
Dianin's compound
Phenol, p-(2,2,4-trimethyl-4-chromanyl)-
4-(4-Hydroxyphenyl)-2,2,4-trimethylchromane
4-(4'-Hydroxyphenyl)-2,2,4-trimethylchroman
4-p-Hydroxyphenyl-2,2,4-trimethylchroman
Chroman I
4-(4-Hydroxyphenyl)-2,2,4-trimethylchroman
2,2,4-Trimethyl-4-(4'-hydroxyphenyl)chroman
NSC 39757
p-(3,4-dihydro-2,2,4-trimethyl-2H-1-benzopyran-4-yl)phenol

Inchi: InChI=1S/C18H20O2/c1-17(2)12-18(3,13-8-10-14(19)11-9-13)15-6-4-5-7-16(15)20-17/h4

InchiKey: KXYDGGNWZUHESZ-UHFFFAOYSA-N

Formula: C18H20O2

SMILES: CC1(C)CC(C)(c2ccc(O)cc2)c2ccccc2O1

Mol. weight [g/mol]: 268.36

Physical Properties

Property code	Value	Unit	Source
hfus	28.34	kJ/mol	Joback Method
logp	4.259		Crippen Method
mcvol	217.840	ml/mol	McGowan Method
tb	639.03	K	Cheméo Relay (1.0)
tf	403.96	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.34	J/mol×K	783.97	Joback Method
cpg	668.16	J/mol×K	828.35	Joback Method
cpg	688.31	J/mol×K	872.72	Joback Method
cpg	709.32	J/mol×K	917.10	Joback Method
cpg	731.70	J/mol×K	961.48	Joback Method
cpg	755.98	J/mol×K	1005.85	Joback Method

cpg	782.67	J/mol×K	1050.23	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C472413&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point