2H-1-Benzopyran-7-ol, 3,4-dihydro-3-(2-hydroxy-4-methoxyphenyl)-

Other names: 3-(2-Hydroxy-4-methoxyphenyl)chroman-7-ol
Inchi: InChI=1S/C16H16O4/c1-19-13-4-5-14(15(18)8-13)11-6-10-2-3-12(17)7-16(10)20-9-11/h2
InchiKey: XRVFNNUXNVWYTI-UHFFFAOYSA-N
Formula: C16H16O4
SMILES: COc1ccc(C2COc3cc(O)ccc3C2)c(O)c1
Mol. weight [g/mol]: 272.30
CAS: 56701-24-7

Physical Properties

Property code	Value	Unit	Source
gf	-162.31	kJ/mol	Joback Method
hf	-475.65	kJ/mol	Joback Method
hfus	41.27	kJ/mol	Joback Method
hvap	90.12	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.825		Crippen Method
mcvol	201.400	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
rinpol	2802.30		NIST Webbook
rinpol	2802.30		NIST Webbook
tb	850.42	K	Joback Method
tc	1110.99	K	Joback Method
tf	634.62	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.76	J/mol×K	850.42	Joback Method
cpg	687.60	J/mol×K	1067.56	Joback Method
cpg	673.67	J/mol×K	1024.14	Joback Method
cpg	659.94	J/mol×K	980.71	Joback Method
cpg	646.20	J/mol×K	937.28	Joback Method
cpg	632.21	J/mol×K	893.85	Joback Method

cpg	701.95	J/mol×K	1110.99	Joback Method
dvisc	0.0000006	Pa×s	850.42	Joback Method
dvisc	0.0000009	Pa×s	814.45	Joback Method
dvisc	0.0000013	Pa×s	778.49	Joback Method
dvisc	0.0000020	Pa×s	742.52	Joback Method
dvisc	0.0000032	Pa×s	706.55	Joback Method
dvisc	0.0000053	Pa×s	670.59	Joback Method
dvisc	0.0000095	Pa×s	634.62	Joback Method

Sources

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=C56701247&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.