(6R,7S,8S)-8-(4-Hydroxy-3-methoxyphenyl)-3-met

Inchi: InChI=1S/C20H24O4/c1-11-7-14-9-19(24-4)17(22)10-15(14)20(12(11)2)13-5-6-16(21)18
InchiKey: TZAAYUCUPIYQBR-UHFFFAOYSA-N
Formula: C20H24O4
SMILES: COc1cc(C2c3cc(O)c(OC)cc3CC(C)C2C)ccc1O
Mol. weight [g/mol]: 328.40
CAS: 36531-08-5

Physical Properties

Property code	Value	Unit	Source
gf	-172.56	kJ/mol	Joback Method
hf	-610.58	kJ/mol	Joback Method
hfus	46.59	kJ/mol	Joback Method
hvap	96.97	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	4.075		Crippen Method
mcvol	257.760	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	2738.30		NIST Webbook
rinpol	2738.30		NIST Webbook
tb	933.05	K	Joback Method
tc	1177.77	K	Joback Method
tf	679.40	K	Joback Method
vc	0.855	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	854.14	J/mol×K	933.05	Joback Method
cpg	871.11	J/mol×K	973.84	Joback Method
cpg	887.44	J/mol×K	1014.62	Joback Method
cpg	903.29	J/mol×K	1055.41	Joback Method
cpg	918.81	J/mol×K	1096.19	Joback Method
cpg	934.16	J/mol×K	1136.98	Joback Method
cpg	949.47	J/mol×K	1177.77	Joback Method

dvisc	0.0000052	Pa×s	679.40	Joback Method
dvisc	0.0000029	Pa×s	721.68	Joback Method
dvisc	0.0000018	Pa×s	763.95	Joback Method
dvisc	0.0000011	Pa×s	806.23	Joback Method
dvisc	0.0000008	Pa×s	848.50	Joback Method
dvisc	0.0000005	Pa×s	890.78	Joback Method
dvisc	0.0000004	Pa×s	933.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36531085&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