6-(1'-Hydroxyethyl)-7-methoxy-2,2-dimethylchrom

Inchi: InChI=1S/C14H18O3/c1-9(15)11-7-10-5-6-14(2,3)17-12(10)8-13(11)16-4/h5-9,15H,1-4H3
InchiKey: ZMQPULSGBXIVGC-UHFFFAOYSA-N
Formula: C14H18O3
SMILES: COc1cc2c(cc1C(C)O)C=CC(C)(C)O2
Mol. weight [g/mol]: 234.29

Physical Properties

Property code	Value	Unit	Source
gf	-106.74	kJ/mol	Joback Method
hf	-412.24	kJ/mol	Joback Method
hfus	25.58	kJ/mol	Joback Method
hvap	73.46	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	2.933		Crippen Method
mcvol	186.810	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
ripol	2545.00		NIST Webbook
ripol	2545.00		NIST Webbook
tb	712.86	K	Joback Method
tc	924.99	K	Joback Method
tf	445.22	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.29	J/mol×K	712.86	Joback Method
cpg	538.29	J/mol×K	748.22	Joback Method
cpg	551.74	J/mol×K	783.57	Joback Method
cpg	564.75	J/mol×K	818.93	Joback Method
cpg	577.44	J/mol×K	854.28	Joback Method
cpg	589.91	J/mol×K	889.64	Joback Method
cpg	602.29	J/mol×K	924.99	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=U360288&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume