Phyllodihydroquinone, 2TMS

Inchi: InChI=1S/C31H48O2/c1-22(2)12-9-13-23(3)14-10-15-24(4)16-11-17-25(5)20-21-27-26(6
InchiKey: BUFJIHPUGZHTHL-JHBCSKSVSA-N
Formula: C31H48O2
SMILES: CC(=CCc1c(C)c(O)c2ccccc2c1O)CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 452.71

Physical Properties

Property code	Value	Unit	Source
gf	165.05	kJ/mol	Joback Method
hf	-541.54	kJ/mol	Joback Method
hfus	66.22	kJ/mol	Joback Method
hvap	114.74	kJ/mol	Joback Method
log10ws	-10.31		Crippen Method
logp	9.487		Crippen Method
mcvol	411.870	ml/mol	McGowan Method
pc	935.77	kPa	Joback Method
rinpol	3487.00		NIST Webbook
rinpol	3487.00		NIST Webbook
tb	1128.26	K	Joback Method
tc	1382.99	K	Joback Method
tf	682.69	K	Joback Method
vc	1.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1504.31	J/mol×K	1128.26	Joback Method
cpg	1533.31	J/mol×K	1170.71	Joback Method
cpg	1563.22	J/mol×K	1213.17	Joback Method
cpg	1594.37	J/mol×K	1255.62	Joback Method
cpg	1627.11	J/mol×K	1298.08	Joback Method
cpg	1661.77	J/mol×K	1340.53	Joback Method
cpg	1698.68	J/mol×K	1382.99	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=R606065&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume