4-Methyl-2-(2-methyltetrahydrofuran-2-yl)phenol

Inchi: InChI=1S/C12H16O2/c1-9-4-5-11(13)10(8-9)12(2)6-3-7-14-12/h4-5,8,13H,3,6-7H2,1-2H3
InchiKey: JNCQVPIRPRPNFS-UHFFFAOYSA-N
Formula: C12H16O2
SMILES: Cc1ccc(O)c(C2(C)CCCO2)c1
Mol. weight [g/mol]: 192.25

Physical Properties

Property code	Value	Unit	Source
gf	-56.74	kJ/mol	Joback Method
hf	-299.54	kJ/mol	Joback Method
hfus	21.89	kJ/mol	Joback Method
hvap	61.87	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.726		Crippen Method
mcvol	157.060	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
rinpol	1629.00		NIST Webbook
tb	628.71	K	Joback Method
tc	879.10	K	Joback Method
tf	437.03	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.52	J/mol×K	628.71	Joback Method
cpg	436.79	J/mol×K	670.44	Joback Method
cpg	452.02	J/mol×K	712.17	Joback Method
cpg	466.45	J/mol×K	753.91	Joback Method
cpg	480.36	J/mol×K	795.64	Joback Method
cpg	494.00	J/mol×K	837.37	Joback Method
cpg	507.62	J/mol×K	879.10	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=R419202&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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