4-methyl-2-tert-butyl-6-hydroperoxymethyl-pheno

Inchi: InChI=1S/C12H18O3/c1-8-5-9(7-15-14)11(13)10(6-8)12(2,3)4/h5-6,13-14H,7H2,1-4H3
InchiKey: FBNSVMKLQJQJDC-UHFFFAOYSA-N
Formula: C12H18O3
SMILES: Cc1cc(COO)c(O)c(C(C)(C)C)c1
Mol. weight [g/mol]: 210.27

Physical Properties

Property code	Value	Unit	Source
gf	-352.38	kJ/mol	Joback Method
hf	-613.75	kJ/mol	Joback Method
hfus	28.61	kJ/mol	Joback Method
hvap	74.79	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.988		Crippen Method
mcvol	173.790	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
rinpol	1614.00		NIST Webbook
rinpol	1614.00		NIST Webbook
tb	733.50	K	Joback Method
tc	967.80	K	Joback Method
tf	551.20	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.50	J/mol×K	733.50	Joback Method
cpg	488.60	J/mol×K	772.55	Joback Method
cpg	499.96	J/mol×K	811.60	Joback Method
cpg	510.72	J/mol×K	850.65	Joback Method
cpg	521.00	J/mol×K	889.70	Joback Method
cpg	530.92	J/mol×K	928.75	Joback Method
cpg	540.60	J/mol×K	967.80	Joback Method
dvisc	0.0001018	Pa×s	551.20	Joback Method

dvisc	0.0000640	Pa×s	581.58	Joback Method
dvisc	0.0000422	Pa×s	611.97	Joback Method
dvisc	0.0000289	Pa×s	642.35	Joback Method
dvisc	0.0000205	Pa×s	672.73	Joback Method
dvisc	0.0000149	Pa×s	703.12	Joback Method
dvisc	0.0000112	Pa×s	733.50	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=R169858&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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