3,4-dihydro-8-hydroxy-4,4,7-trimethyl-2(1H)-napht

Inchi: InChI=1S/C13H16O2/c1-8-4-5-11-10(12(8)15)6-9(14)7-13(11,2)3/h4-5,15H,6-7H2,1-3H3
InchiKey: BDNLGQMIYVVUJE-UHFFFAOYSA-N
Formula: C13H16O2
SMILES: Cc1ccc2c(c1O)CC(=O)CC2(C)C
Mol. weight [g/mol]: 204.26

Physical Properties

Property code	Value	Unit	Source
gf	-82.32	kJ/mol	Joback Method
hf	-331.19	kJ/mol	Joback Method
hfus	17.72	kJ/mol	Joback Method
hvap	64.33	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.494		Crippen Method
mcvol	166.850	ml/mol	McGowan Method
pc	3152.62	kPa	Joback Method
rinpol	1668.00		NIST Webbook
tb	693.17	K	Joback Method
tc	946.04	K	Joback Method
tf	505.99	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.74	J/mol×K	693.17	Joback Method
cpg	480.76	J/mol×K	735.32	Joback Method
cpg	496.14	J/mol×K	777.46	Joback Method
cpg	511.10	J/mol×K	819.61	Joback Method
cpg	525.87	J/mol×K	861.75	Joback Method
cpg	540.68	J/mol×K	903.90	Joback Method
cpg	555.75	J/mol×K	946.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R288810&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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