

campherenol

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H26O/c1-11(2)6-5-8-14(3)12-7-9-15(14,4)13(16)10-12/h6,12-13,16H,5,7-1

SGAYOTORECIFCJ-IBLUKRHDSA-N

C15H26O

CC(C)=CCCC1(C)C2CCC1(C)C(O)C2

222.37

Physical Properties

Property code	Value	Unit	Source
gf	93.27	kJ/mol	Joback Method
hf	-268.49	kJ/mol	Joback Method
hfus	21.30	kJ/mol	Joback Method
hvap	62.78	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.920		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	1654.00		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1680.00		NIST Webbook
ripol	2245.00		NIST Webbook
tb	647.71	K	Joback Method
tc	846.27	K	Joback Method
tf	372.27	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	587.48	J/mol×K	647.71	Joback Method
cpg	605.51	J/mol×K	680.80	Joback Method
cpg	622.77	J/mol×K	713.90	Joback Method
cpg	639.47	J/mol×K	746.99	Joback Method

cpg	655.81	J/mol×K	780.09	Joback Method
cpg	672.00	J/mol×K	813.18	Joback Method
cpg	688.24	J/mol×K	846.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R235504&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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