«beta»-Acoradienol

Inchi: InChI=1S/C15H24O/c1-11(2)14-5-4-12(3)15(14)8-6-13(10-16)7-9-15/h6,12,14,16H,1,4-5
InchiKey: KBMDEJULGPFFGC-UHFFFAOYSA-N
Formula: C15H24O
SMILES: C=C(C)C1CCC(C)C12CC=C(CO)CC2
Mol. weight [g/mol]: 220.35
CAS: 149496-35-5

Physical Properties

Property code	Value	Unit	Source
gf	98.12	kJ/mol	Joback Method
hf	-227.35	kJ/mol	Joback Method
hfus	19.58	kJ/mol	Joback Method
hvap	65.08	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.698		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2212.45	kPa	Joback Method
rinpol	1736.00		NIST Webbook
rinpol	1732.00		NIST Webbook
rinpol	1732.00		NIST Webbook
rinpol	1732.00		NIST Webbook
rinpol	1732.00		NIST Webbook
rinpol	1736.00		NIST Webbook
rinpol	1754.00		NIST Webbook
rinpol	1764.10		NIST Webbook
rinpol	1768.00		NIST Webbook
rinpol	1741.00		NIST Webbook
rinpol	1757.00		NIST Webbook
tb	661.61	K	Joback Method
tc	869.92	K	Joback Method
tf	358.65	K	Joback Method
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.16	J/mol×K	661.61	Joback Method
cpg	591.06	J/mol×K	696.33	Joback Method
cpg	608.99	J/mol×K	731.05	Joback Method
cpg	626.07	J/mol×K	765.76	Joback Method
cpg	642.44	J/mol×K	800.48	Joback Method
cpg	658.24	J/mol×K	835.20	Joback Method
cpg	673.58	J/mol×K	869.92	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C149496355&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