«alpha»-Isonootkatol

Inchi: InChI=1S/C15H24O/c1-10(2)12-5-6-13-8-14(16)7-11(3)15(13,4)9-12/h8,11,14,16H,5-7,9
InchiKey: OKGZNXMPKYHFRT-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CC(C)=C1CCC2=CC(O)CC(C)C2(C)C1
Mol. weight [g/mol]: 220.35
CAS: 1380573-94-3

Physical Properties

Property code	Value	Unit	Source
gf	55.74	kJ/mol	Joback Method
hf	-276.75	kJ/mol	Joback Method
hfus	21.18	kJ/mol	Joback Method
hvap	66.54	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.840		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2185.64	kPa	Joback Method
rinpol	2405.40		NIST Webbook
rinpol	2405.40		NIST Webbook
tb	671.57	K	Joback Method
tc	881.76	K	Joback Method
tf	370.77	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.72	J/mol×K	671.57	Joback Method
cpg	591.29	J/mol×K	706.60	Joback Method
cpg	608.94	J/mol×K	741.63	Joback Method
cpg	625.83	J/mol×K	776.66	Joback Method
cpg	642.07	J/mol×K	811.69	Joback Method
cpg	657.79	J/mol×K	846.72	Joback Method
cpg	673.14	J/mol×K	881.76	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1380573943&Units=SI

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

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