

Isohumbertiol B

Inchi:	InChI=1S/C15H26O/c1-6-15(5,16)10-13-9-12(4)7-8-14(13)11(2)3/h6,9,11,13-14,16H,1,7
InchiKey:	YDECUWOATDRFNP-FGRDXJNISA-N
Formula:	C15H26O
SMILES:	C=CC(C)(O)CC1C=C(C)CCC1C(C)C
Mol. weight [g/mol]:	222.37

Physical Properties

Property code	Value	Unit	Source
gf	63.91	kJ/mol	Joback Method
hf	-313.47	kJ/mol	Joback Method
hfus	20.22	kJ/mol	Joback Method
hvap	64.38	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.942		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	1883.80	kPa	Joback Method
ripol	1522.00		NIST Webbook
ripol	2032.00		NIST Webbook
ripol	2032.00		NIST Webbook
tb	646.81	K	Joback Method
tc	841.23	K	Joback Method
tf	321.71	K	Joback Method
vc	0.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.43	J/molxK	646.81	Joback Method
cpg	673.00	J/molxK	808.82	Joback Method
cpg	658.42	J/molxK	776.42	Joback Method
cpg	642.92	J/molxK	744.02	Joback Method
cpg	626.45	J/molxK	711.62	Joback Method
cpg	608.97	J/molxK	679.21	Joback Method
cpg	686.70	J/molxK	841.23	Joback Method

dvisc	0.0000519	Paxs	646.81	Joback Method
dvisc	0.0000837	Paxs	592.63	Joback Method
dvisc	0.0001487	Paxs	538.44	Joback Method
dvisc	0.0003005	Paxs	484.26	Joback Method
dvisc	0.0007249	Paxs	430.08	Joback Method
dvisc	0.0022543	Paxs	375.89	Joback Method
dvisc	0.0102738	Paxs	321.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R232689&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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