Isohumbertiol A

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-DMJDIKPUSA-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
rinpol	1495.00		NIST Webbook
ripol	2006.00		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/mol×K	646.81	Joback Method
cpg	608.97	J/mol×K	679.21	Joback Method
cpg	626.45	J/mol×K	711.62	Joback Method
cpg	642.92	J/mol×K	744.02	Joback Method
cpg	658.42	J/mol×K	776.42	Joback Method
cpg	673.00	J/mol×K	808.82	Joback Method
cpg	686.70	J/mol×K	841.23	Joback Method
dvisc	0.0102738	Pa×s	321.71	Joback Method

dvisc	0.0022543	Pa×s	375.89	Joback Method
dvisc	0.0007249	Pa×s	430.08	Joback Method
dvisc	0.0003005	Pa×s	484.26	Joback Method
dvisc	0.0001487	Pa×s	538.44	Joback Method
dvisc	0.0000837	Pa×s	592.63	Joback Method
dvisc	0.0000519	Pa×s	646.81	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=R232674&Units=SI

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