Vomifoliol

Other names: Blumenol A
Inchi: InChI=1S/C13H20O3/c1-9-7-11(15)8-12(3,4)13(9,16)6-5-10(2)14/h5-7,10,14,16H,8H2,1-
InchiKey: KPQMCAKZRXOZLB-BXQPDHIASA-N
Formula: C13H20O3
SMILES: CC1=CC(=O)CC(C)(C)C1(O)C=CC(C)O
Mol. weight [g/mol]: 224.30
CAS: 23526-45-6

Physical Properties

Property code	Value	Unit	Source
gf	-233.78	kJ/mol	Joback Method
hf	-531.10	kJ/mol	Joback Method
hfus	14.93	kJ/mol	Joback Method
hvap	80.48	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	1.600		Crippen Method
mcvol	187.880	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
rinpol	1806.00		NIST Webbook
rinpol	1806.00		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1814.00		NIST Webbook
rinpol	1772.00		NIST Webbook
rinpol	1774.00		NIST Webbook
rinpol	1772.00		NIST Webbook
rinpol	1778.00		NIST Webbook
rinpol	1769.00		NIST Webbook
rinpol	1796.00		NIST Webbook
rinpol	1794.00		NIST Webbook
rinpol	1796.00		NIST Webbook
ripol	3167.00		NIST Webbook
ripol	3128.00		NIST Webbook
ripol	3175.00		NIST Webbook
ripol	3170.00		NIST Webbook
ripol	3128.00		NIST Webbook
ripol	3170.00		NIST Webbook
ripol	3175.00		NIST Webbook

ripol	3192.00		NIST Webbook
ripol	3131.00		NIST Webbook
ripol	3200.00		NIST Webbook
ripol	3192.00		NIST Webbook
ripol	3167.00		NIST Webbook
ripol	3167.00		NIST Webbook
ripol	3167.00		NIST Webbook
ripol	3170.00		NIST Webbook
ripol	3175.00		NIST Webbook
tb	772.24	K	Joback Method
tc	978.61	K	Joback Method
tf	470.27	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.30	J/mol×K	772.24	Joback Method
cpg	582.00	J/mol×K	806.64	Joback Method
cpg	596.66	J/mol×K	841.03	Joback Method
cpg	611.44	J/mol×K	875.43	Joback Method
cpg	626.50	J/mol×K	909.82	Joback Method
cpg	642.00	J/mol×K	944.22	Joback Method
cpg	658.11	J/mol×K	978.61	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C23526456&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

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