bornyl benzoate

Inchi: InChI=1S/C17H22O2/c1-16(2)13-9-10-17(16,3)14(11-13)19-15(18)12-7-5-4-6-8-12/h4-8,
InchiKey: FLOISDYCXINJOB-KEYYUXOJSA-N
Formula: C17H22O2
SMILES: CC1(C)C2CCC1(C)C(OC(=O)c1ccccc1)C2
Mol. weight [g/mol]: 258.36

Physical Properties

Property code	Value	Unit	Source
gf	53.75	kJ/mol	Joback Method
hf	-273.24	kJ/mol	Joback Method
hfus	20.33	kJ/mol	Joback Method
hvap	61.95	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.058		Crippen Method
mcvol	212.350	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
rinpol	1749.00		NIST Webbook
rinpol	1749.00		NIST Webbook
rinpol	1749.00		NIST Webbook
tb	700.22	K	Joback Method
tc	939.44	K	Joback Method
tf	451.61	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.43	J/mol×K	700.22	Joback Method
cpg	644.92	J/mol×K	740.09	Joback Method
cpg	664.64	J/mol×K	779.96	Joback Method
cpg	683.94	J/mol×K	819.83	Joback Method
cpg	703.13	J/mol×K	859.70	Joback Method
cpg	722.54	J/mol×K	899.57	Joback Method
cpg	742.50	J/mol×K	939.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R204847&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