Bornyl tiglate

Inchi: InChI=1S/C15H24O2/c1-6-10(2)13(16)17-12-9-11-7-8-15(12,5)14(11,3)4/h6,11-12H,7-9H
InchiKey: ZUVAGNOBOHVXJJ-UXBLZVDNSA-N
Formula: C15H24O2
SMILES: CC=C(C)C(=O)OC1CC2CCC1(C)C2(C)C
Mol. weight [g/mol]: 236.35
CAS: 101223-92-1

Physical Properties

Property code	Value	Unit	Source
gf	-3.83	kJ/mol	Joback Method
hf	-361.06	kJ/mol	Joback Method
hfus	20.00	kJ/mol	Joback Method
hvap	55.26	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.711		Crippen Method
mcvol	203.630	ml/mol	McGowan Method
pc	1982.35	kPa	Joback Method
rinpol	1615.40		NIST Webbook
tb	631.82	K	Joback Method
tc	849.20	K	Joback Method
tf	383.61	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.31	J/mol×K	631.82	Joback Method
cpg	592.10	J/mol×K	668.05	Joback Method
cpg	610.91	J/mol×K	704.28	Joback Method
cpg	628.99	J/mol×K	740.51	Joback Method
cpg	646.59	J/mol×K	776.74	Joback Method
cpg	663.95	J/mol×K	812.97	Joback Method
cpg	681.31	J/mol×K	849.20	Joback Method

Sources

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=C101223921&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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