Triquinacene, 1,4-bis(methoxy)-

Inchi: InChI=1S/C12H14O2/c1-13-11-5-3-9-4-6-12(14-2,8-7-11)10(9)11/h3-10H,1-2H3
InchiKey: VBJAIPBIFMKJQV-UHFFFAOYSA-N
Formula: C12H14O2
SMILES: COC12C=CC3C=CC(OC)(C=C1)C32
Mol. weight [g/mol]: 190.24
CAS: 60958-96-5

Physical Properties

Property code	Value	Unit	Source
gf	81.50	kJ/mol	Joback Method
hf	-159.73	kJ/mol	Joback Method
hfus	13.66	kJ/mol	Joback Method
hvap	45.30	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	1.699		Crippen Method
mcvol	146.200	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
rinpol	1641.00		NIST Webbook
tb	536.58	K	Joback Method
tc	764.26	K	Joback Method
tf	365.60	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.71	J/mol×K	536.58	Joback Method
cpg	386.48	J/mol×K	574.53	Joback Method
cpg	401.82	J/mol×K	612.47	Joback Method
cpg	416.04	J/mol×K	650.42	Joback Method
cpg	429.40	J/mol×K	688.37	Joback Method
cpg	442.21	J/mol×K	726.32	Joback Method
cpg	454.73	J/mol×K	764.26	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=C60958965&Units=SI

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