Triquinacene, 1,4,7-tris(methoxy)-

Inchi: InChI=1S/C13H16O3/c1-14-11-4-6-12(15-2)8-9-13(16-3,7-5-11)10(11)12/h4-10H,1-3H3
InchiKey: CEKGUCISQAISMC-UHFFFAOYSA-N
Formula: C13H16O3
SMILES: COC12C=CC3(OC)C=CC(OC)(C=C1)C23
Mol. weight [g/mol]: 220.26
CAS: 60958-97-6

Physical Properties

Property code	Value	Unit	Source
gf	-20.57	kJ/mol	Joback Method
hf	-297.35	kJ/mol	Joback Method
hfus	11.14	kJ/mol	Joback Method
hvap	48.79	kJ/mol	Joback Method
log10ws	-1.87		Crippen Method
logp	1.468		Crippen Method
mcvol	166.160	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
rinpol	1827.00		NIST Webbook
tb	582.12	K	Joback Method
tc	811.80	K	Joback Method
tf	423.00	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.72	J/mol×K	582.12	Joback Method
cpg	458.02	J/mol×K	620.40	Joback Method
cpg	473.22	J/mol×K	658.68	Joback Method
cpg	487.71	J/mol×K	696.96	Joback Method
cpg	501.85	J/mol×K	735.24	Joback Method
cpg	516.04	J/mol×K	773.52	Joback Method
cpg	530.64	J/mol×K	811.80	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=C60958976&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