Porosa-4,6-dien-7-one

Inchi: InChI=1S/C15H22O/c1-10(2)14(16)12-8-13-11(3)6-5-7-15(13,4)9-12/h8,10H,5-7,9H2,1-4
InchiKey: AUHXWVNWVPJIJR-OAHLLOKOSA-N
Formula: C15H22O
SMILES: CC1=C2C=C(C(=O)C(C)C)CC2(C)CCC1
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	62.51	kJ/mol	Joback Method
hf	-226.94	kJ/mol	Joback Method
hfus	16.56	kJ/mol	Joback Method
hvap	57.41	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.048		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2169.38	kPa	Joback Method
rinpol	1657.00		NIST Webbook
rinpol	1657.00		NIST Webbook
tb	640.49	K	Joback Method
tc	865.05	K	Joback Method
tf	386.28	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.26	J/mol×K	640.49	Joback Method
cpg	541.85	J/mol×K	677.92	Joback Method
cpg	559.40	J/mol×K	715.34	Joback Method
cpg	576.09	J/mol×K	752.77	Joback Method
cpg	592.08	J/mol×K	790.20	Joback Method
cpg	607.54	J/mol×K	827.62	Joback Method
cpg	622.62	J/mol×K	865.05	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=R199210&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