(-)-3 «beta»,4 «beta»-oxidoagarofuran

Other names: 3 «beta»,4 «beta»-Oxydoagarofuran
Inchi: InChI=1S/C15H24O2/c1-12(2)10-5-7-13(3)8-6-11-14(4,16-11)15(13,9-10)17-12/h10-11H
InchiKey: SMVQLPPNRFDHMB-QFCKPIOYSA-N
Formula: C15H24O2
SMILES: CC1(C)OC23CC1CCC2(C)CCC1OC13C
Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
gf	96.70	kJ/mol	Joback Method
hf	-311.61	kJ/mol	Joback Method
hfus	17.95	kJ/mol	Joback Method
hvap	52.61	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.292		Crippen Method
mcvol	190.510	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
rinpol	1685.00		NIST Webbook
ripol	2282.00		NIST Webbook
ripol	2322.00		NIST Webbook
tb	619.35	K	Joback Method
tc	863.34	K	Joback Method
tf	467.31	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.87	J/mol×K	619.35	Joback Method
cpg	595.50	J/mol×K	660.01	Joback Method
cpg	615.99	J/mol×K	700.68	Joback Method
cpg	635.99	J/mol×K	741.34	Joback Method
cpg	656.19	J/mol×K	782.01	Joback Method
cpg	677.24	J/mol×K	822.67	Joback Method

cpg	699.82	J/mol×K	863.34	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=R342875&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume