1,10-seco-Aromadendran-1,10-dione

Inchi: InChI=1S/C15H24O2/c1-9-5-8-12(17)13(9)14-11(15(14,3)4)7-6-10(2)16/h9,11,13-14H,5-
InchiKey: ZIRTVHDRHVNBGO-VMXABPDPSA-N
Formula: C15H24O2
SMILES: CC(=O)CCC1C(C2C(=O)CCC2C)C1(C)C
Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
gf	-107.41	kJ/mol	Joback Method
hf	-515.71	kJ/mol	Joback Method
hfus	24.70	kJ/mol	Joback Method
hvap	58.07	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	3.243		Crippen Method
mcvol	203.630	ml/mol	McGowan Method
pc	1883.80	kPa	Joback Method
rinpol	1707.00		NIST Webbook
rinpol	1707.00		NIST Webbook
ripol	2448.00		NIST Webbook
ripol	2448.00		NIST Webbook
tb	672.54	K	Joback Method
tc	890.95	K	Joback Method
tf	416.98	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.47	J/mol×K	672.54	Joback Method
cpg	631.53	J/mol×K	708.94	Joback Method
cpg	651.55	J/mol×K	745.34	Joback Method
cpg	670.62	J/mol×K	781.75	Joback Method
cpg	688.87	J/mol×K	818.15	Joback Method
cpg	706.40	J/mol×K	854.55	Joback Method

cpg	723.35	J/mol×K	890.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R228650&Units=SI
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

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