African-1(5)-en-2,6-dione

Inchi: InChI=1S/C15H20O2/c1-8-5-10(16)12-11(8)13(17)14(2,3)6-9-7-15(9,12)4/h8-9H,5-7H2,1
InchiKey: PUPACQJMSZEBOJ-QWTSGDGFSA-N
Formula: C15H20O2
SMILES: CC1CC(=O)C2=C1C(=O)C(C)(C)CC1CC21C
Mol. weight [g/mol]: 232.32

Physical Properties

Property code	Value	Unit	Source
gf	-19.70	kJ/mol	Joback Method
hf	-377.27	kJ/mol	Joback Method
hfus	12.75	kJ/mol	Joback Method
hvap	56.57	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.917		Crippen Method
mcvol	188.470	ml/mol	McGowan Method
pc	2300.32	kPa	Joback Method
rinpol	1644.00		NIST Webbook
rinpol	1644.00		NIST Webbook
tb	711.93	K	Joback Method
tc	962.62	K	Joback Method
tf	511.39	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.69	J/mol×K	711.93	Joback Method
cpg	596.40	J/mol×K	753.71	Joback Method
cpg	616.60	J/mol×K	795.49	Joback Method
cpg	636.59	J/mol×K	837.27	Joback Method
cpg	656.67	J/mol×K	879.05	Joback Method
cpg	677.15	J/mol×K	920.84	Joback Method
cpg	698.35	J/mol×K	962.62	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=R421215&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume