Silphiperfol-6-en-3,5-dione

Inchi: InChI=1S/C15H20O2/c1-8-5-6-15-10(3)9(2)13(17)14(15,4)12(16)7-11(8)15/h8,11H,5-7H2
InchiKey: LUEUBVVPFGOSDR-BXLXJPJESA-N
Formula: C15H20O2
SMILES: CC1=C(C)C23CCC(C)C2CC(=O)C3(C)C1=O
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	1651.00		NIST Webbook
rinpol	1651.00		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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R226892&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume