Cyperadione

Inchi: InChI=1S/C15H24O2/c1-10-5-6-12-9-13(17)15(10,14(12,3)4)8-7-11(2)16/h10,12H,5-9H2
InchiKey: JNYTXKVQDFVROJ-UHFFFAOYSA-N
Formula: C15H24O2
SMILES: CC(=O)CCC12C(=O)CC(CCC1C)C2(C)C
Mol. weight [g/mol]: 236.35
CAS: 394656-12-3

Physical Properties

Property code	Value	Unit	Source
gf	-105.19	kJ/mol	Joback Method
hf	-480.13	kJ/mol	Joback Method
hfus	17.33	kJ/mol	Joback Method
hvap	57.23	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.387		Crippen Method
mcvol	203.630	ml/mol	McGowan Method
pc	2018.13	kPa	Joback Method
rinpol	1844.80		NIST Webbook
tb	677.45	K	Joback Method
tc	903.66	K	Joback Method
tf	445.12	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.71	J/mol×K	677.45	Joback Method
cpg	625.38	J/mol×K	715.15	Joback Method
cpg	645.25	J/mol×K	752.85	Joback Method
cpg	664.57	J/mol×K	790.56	Joback Method
cpg	683.56	J/mol×K	828.26	Joback Method
cpg	702.46	J/mol×K	865.96	Joback Method
cpg	721.49	J/mol×K	903.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C394656123&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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