Muurol-4-en-3,8-dione

Inchi: InChI=1S/C15H22O2/c1-8(2)15-12-5-10(4)13(16)7-11(12)9(3)6-14(15)17/h5,8-9,11-12,15
InchiKey: CUTPLKRCZNTUMR-CIPDSAHDSA-N
Formula: C15H22O2
SMILES: CC1=CC2C(CC1=O)C(C)CC(=O)C2C(C)C
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	-94.19	kJ/mol	Joback Method
hf	-507.02	kJ/mol	Joback Method
hfus	20.95	kJ/mol	Joback Method
hvap	57.94	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	3.019		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
pc	1949.23	kPa	Joback Method
rinpol	1784.00		NIST Webbook
rinpol	1784.00		NIST Webbook
tb	703.16	K	Joback Method
tc	939.59	K	Joback Method
tf	406.85	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.67	J/mol×K	703.16	Joback Method
cpg	630.97	J/mol×K	742.56	Joback Method
cpg	651.72	J/mol×K	781.97	Joback Method
cpg	670.90	J/mol×K	821.37	Joback Method
cpg	688.49	J/mol×K	860.78	Joback Method
cpg	704.46	J/mol×K	900.18	Joback Method
cpg	718.80	J/mol×K	939.59	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=R227117&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