isovalencenal

Inchi: InChI=1S/C15H22O/c1-11(10-16)13-7-8-14-6-4-5-12(2)15(14,3)9-13/h6,9-12H,4-5,7-8H2
InchiKey: OYMZYJHDWGJMHB-WQKBPTQTSA-N
Formula: C15H22O
SMILES: CC(C=O)C1=CC2(C)C(=CCCC2C)CC1
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	81.73	kJ/mol	Joback Method
hf	-214.97	kJ/mol	Joback Method
hfus	16.61	kJ/mol	Joback Method
hvap	56.59	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.904		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2206.22	kPa	Joback Method
ripol	2453.00		NIST Webbook
tb	629.90	K	Joback Method
tc	856.00	K	Joback Method
tf	358.07	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.24	J/mol×K	629.90	Joback Method
cpg	547.12	J/mol×K	667.58	Joback Method
cpg	565.84	J/mol×K	705.27	Joback Method
cpg	583.54	J/mol×K	742.95	Joback Method
cpg	600.38	J/mol×K	780.63	Joback Method
cpg	616.52	J/mol×K	818.32	Joback Method
cpg	632.14	J/mol×K	856.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R341238&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume