«beta»-(Z)-Elemenone

Inchi: InChI=1S/C15H22O/c1-7-15(6)9-14(16)12(10(2)3)8-13(15)11(4)5/h7,13H,1,4,8-9H2,2-3,5
InchiKey: ABLPGPHZENVRRH-ZFWWWQNUSA-N
Formula: C15H22O
SMILES: C=CC1(C)CC(=O)C(=C(C)C)CC1C(=C)C
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	168.12	kJ/mol	Joback Method
hf	-134.10	kJ/mol	Joback Method
hfus	15.87	kJ/mol	Joback Method
hvap	51.81	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.070		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	1918.62	kPa	Joback Method
rinpol	1580.00		NIST Webbook
rinpol	1580.00		NIST Webbook
tb	625.30	K	Joback Method
tc	852.13	K	Joback Method
tf	332.99	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	529.91	J/mol×K	625.30	Joback Method
cpg	550.52	J/mol×K	663.11	Joback Method
cpg	570.03	J/mol×K	700.91	Joback Method
cpg	588.56	J/mol×K	738.72	Joback Method
cpg	606.24	J/mol×K	776.52	Joback Method
cpg	623.19	J/mol×K	814.33	Joback Method
cpg	639.53	J/mol×K	852.13	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=R616849&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