6-Epishyobunone

Inchi: InChI=1S/C15H24O/c1-7-15(6)9-8-12(10(2)3)14(16)13(15)11(4)5/h7,10,12-13H,1,4,8-9H
InchiKey: GWHRSRIPLDHJHR-NFAWXSAZSA-N
Formula: C15H24O
SMILES: C=CC1(C)CCC(C(C)C)C(=O)C1C(=C)C
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	121.06	kJ/mol	Joback Method
hf	-225.96	kJ/mol	Joback Method
hfus	14.40	kJ/mol	Joback Method
hvap	50.24	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	4.006		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	1823.17	kPa	Joback Method
rinpol	1480.00		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1482.00		NIST Webbook
ripol	1854.00		NIST Webbook
ripol	1846.00		NIST Webbook
ripol	1846.00		NIST Webbook
tb	613.67	K	Joback Method
tc	834.59	K	Joback Method
tf	317.35	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.57	J/mol×K	613.67	Joback Method
cpg	574.78	J/mol×K	650.49	Joback Method
cpg	595.82	J/mol×K	687.31	Joback Method

cpg	615.78	J/mol×K	724.13	Joback Method
cpg	634.76	J/mol×K	760.95	Joback Method
cpg	652.87	J/mol×K	797.77	Joback Method
cpg	670.21	J/mol×K	834.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R406345&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume