Shyobunone isomer 2

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-PIMMBPRGSA-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	1510.00		NIST Webbook
rinpol	1510.00		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

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=R518953&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

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