Norbourbonone

Other names: 1-nor-Bourbonanone
Bourbonanone <1-nor
Inchi: InChI=1S/C14H22O/c1-8(2)9-6-7-14(3)10-4-5-11(15)12(10)13(9)14/h8-10,12-13H,4-7H2
InchiKey: PYUWACLOPFTHBV-UHFFFAOYSA-N
Formula: C14H22O
SMILES: CC(C)C1CCC2(C)C3CCC(=O)C3C12
Mol. weight [g/mol]: 206.32
CAS: 13844-03-6

Physical Properties

Property code	Value	Unit	Source
gf	91.21	kJ/mol	Joback Method
hf	-288.47	kJ/mol	Joback Method
hfus	16.15	kJ/mol	Joback Method
hvap	48.76	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	3.284		Crippen Method
mcvol	177.110	ml/mol	McGowan Method
pc	2214.53	kPa	Joback Method
rinpol	1599.00		NIST Webbook
rinpol	1568.00		NIST Webbook
rinpol	1548.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1571.40		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1563.00		NIST Webbook
rinpol	1563.00		NIST Webbook
rinpol	1563.00		NIST Webbook
rinpol	1568.00		NIST Webbook
rinpol	1558.00		NIST Webbook
rinpol	1571.40		NIST Webbook
ripol	2046.00		NIST Webbook
ripol	2045.00		NIST Webbook
ripol	2045.00		NIST Webbook
ripol	2046.00		NIST Webbook
ripol	2046.00		NIST Webbook
ripol	2046.00		NIST Webbook

tb	602.49	K	Joback Method
tc	830.61	K	Joback Method
tf	366.48	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.78	J/mol×K	602.49	Joback Method
cpg	534.11	J/mol×K	640.51	Joback Method
cpg	555.07	J/mol×K	678.53	Joback Method
cpg	574.84	J/mol×K	716.55	Joback Method
cpg	593.60	J/mol×K	754.57	Joback Method
cpg	611.55	J/mol×K	792.59	Joback Method
cpg	628.85	J/mol×K	830.61	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13844036&Units=SI

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