Bicyclo[3.1.0]hexan-2-one, 1,5-bis(1,1-dimethylethyl)-3,3-dimethyl-

Other names: Bicyclo[3.1.0]hexan-2-one, 1,5-di-tert-butyl-3,3-dimethyl-
1,5-Ditert-butyl-3,3-dimethylbicyclo[3.1.0]hexan-2-one
1,5-bis(1,1-Dimethylethyl)-3,3-dimethyl-bicyclo[3.1.0]hexan-2-one
Bicyclo[3.1.0]hexan-2-one, 1,5-bis-tert.-butyl-3,3-dimethyl

Inchi: InChI=1S/C16H28O/c1-12(2,3)15-9-14(7,8)11(17)16(15,10-15)13(4,5)6/h9-10H2,1-8H3

InchiKey: BPSOBKPRRBSNAW-UHFFFAOYSA-N

Formula: C16H28O

SMILES: CC1(C)CC2(C(C)(C)C)CC2(C(C)(C)C)C1=O

Mol. weight [g/mol]: 236.39

CAS: 19377-95-8

Physical Properties

Property code	Value	Unit	Source
gf	64.25	kJ/mol	Joback Method
hf	-357.79	kJ/mol	Joback Method
hfus	0.33	kJ/mol	Joback Method
hvap	48.93	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	4.454		Crippen Method
mcvol	216.150	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
rinpol	1565.00		NIST Webbook
rinpol	1565.00		NIST Webbook
ripol	2108.00		NIST Webbook
ripol	2073.00		NIST Webbook
ripol	2073.00		NIST Webbook
tb	636.37	K	Joback Method
tc	872.21	K	Joback Method
tf	446.48	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	628.86	J/mol×K	636.37	Joback Method
cpg	650.92	J/mol×K	675.68	Joback Method
cpg	671.91	J/mol×K	714.98	Joback Method
cpg	692.29	J/mol×K	754.29	Joback Method
cpg	712.54	J/mol×K	793.60	Joback Method
cpg	733.10	J/mol×K	832.91	Joback Method
cpg	754.46	J/mol×K	872.21	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=C19377958&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume