

8,9,10-trinorborn-5-ene-2-spiro-1'-(2'-isobutyroxy)

Inchi:	InChI=1S/C16H24O2/c1-11(2)15(17)18-14-5-3-4-8-16(14)10-12-6-7-13(16)9-12/h6-7,11-
InchiKey:	FCEVUWZGSPSHNE-UHFFFAOYSA-N
Formula:	C16H24O2
SMILES:	CC(C)C(=O)OC1CCCCC12CC1C=CC2C1
Mol. weight [g/mol]:	248.36

Physical Properties

Property code	Value	Unit	Source
gf	10.19	kJ/mol	Joback Method
hf	-371.05	kJ/mol	Joback Method
hfus	20.56	kJ/mol	Joback Method
hvap	59.06	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.711		Crippen Method
mcvol	206.860	ml/mol	McGowan Method
pc	2090.75	kPa	Joback Method
ripol	1707.40		NIST Webbook
ripol	1714.70		NIST Webbook
ripol	1707.40		NIST Webbook
ripol	2121.80		NIST Webbook
ripol	2130.00		NIST Webbook
ripol	2121.80		NIST Webbook
tb	669.09	K	Joback Method
tc	896.78	K	Joback Method
tf	390.92	K	Joback Method
vc	0.779	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.51	J/molxK	669.09	Joback Method
cpg	640.24	J/molxK	707.04	Joback Method
cpg	660.69	J/molxK	744.99	Joback Method
cpg	680.08	J/molxK	782.93	Joback Method

cpg	698.59	J/mol×K	820.88	Joback Method
cpg	716.42	J/mol×K	858.83	Joback Method
cpg	733.77	J/mol×K	896.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R327792&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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