1,5,5-trimethyl-9-oxabicyclo[4.3]non-6-en-3-one

Inchi: InChI=1S/C11H16O2/c1-10(2)6-8(12)7-11(3)9(10)4-5-13-11/h4H,5-7H2,1-3H3
InchiKey: XSBKKKQUAMYPAW-UHFFFAOYSA-N
Formula: C11H16O2
SMILES: CC1(C)CC(=O)CC2(C)OCC=C12
Mol. weight [g/mol]: 180.24

Physical Properties

Property code	Value	Unit	Source
gf	-72.42	kJ/mol	Joback Method
hf	-336.16	kJ/mol	Joback Method
hfus	9.94	kJ/mol	Joback Method
hvap	47.83	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.091		Crippen Method
mcvol	147.270	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
rinpol	1500.00		NIST Webbook
rinpol	1500.00		NIST Webbook
ripol	2090.00		NIST Webbook
ripol	2090.00		NIST Webbook
tb	576.76	K	Joback Method
tc	823.41	K	Joback Method
tf	394.92	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.12	J/mol×K	576.76	Joback Method
cpg	401.95	J/mol×K	617.87	Joback Method
cpg	418.65	J/mol×K	658.98	Joback Method
cpg	434.48	J/mol×K	700.08	Joback Method
cpg	449.74	J/mol×K	741.19	Joback Method
cpg	464.70	J/mol×K	782.30	Joback Method

cpg	479.66	J/mol×K	823.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R149196&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

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