

3,3-Dimethyl-2-norbornanone dimethyl ketal

Inchi:	InChI=1S/C11H20O2/c1-10(2)8-5-6-9(7-8)11(10,12-3)13-4/h8-9H,5-7H2,1-4H3
InchiKey:	PYJMUZABCPLHBD-UHFFFAOYSA-N
Formula:	C11H20O2
SMILES:	COC1(OC)C2CCC(C2)C1(C)C
Mol. weight [g/mol]:	184.28
CAS:	124287-82-7

Physical Properties

Property code	Value	Unit	Source
gf	-85.26	kJ/mol	Joback Method
hf	-405.57	kJ/mol	Joback Method
hfus	10.34	kJ/mol	Joback Method
hvap	58.32	kJ/mol	NIST Webbook
log10ws	-2.27		Crippen Method
logp	2.432		Crippen Method
mcvol	155.870	ml/mol	McGowan Method
pc	2502.50	kPa	Joback Method
tb	504.81	K	Joback Method
tc	712.90	K	Joback Method
tf	329.87	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.26	J/molxK	504.81	Joback Method
cpg	409.58	J/molxK	539.49	Joback Method
cpg	427.60	J/molxK	574.17	Joback Method
cpg	444.50	J/molxK	608.86	Joback Method
cpg	460.47	J/molxK	643.54	Joback Method
cpg	475.69	J/molxK	678.22	Joback Method
cpg	490.33	J/molxK	712.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C124287827&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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