1,7,7-Trimethyl-2-norbornanone dimethyl ketal

Inchi: InChI=1S/C12H22O2/c1-10(2)9-6-7-11(10,3)12(8-9,13-4)14-5/h9H,6-8H2,1-5H3
InchiKey: RRCYFCPKYNYACP-UHFFFAOYSA-N
Formula: C12H22O2
SMILES: COC1(OC)CC2CCC1(C)C2(C)C
Mol. weight [g/mol]: 198.30
CAS: 10395-50-3

Physical Properties

Property code	Value	Unit	Source
gf	-82.33	kJ/mol	Joback Method
hf	-410.97	kJ/mol	Joback Method
hfus	6.63	kJ/mol	Joback Method
hvap	61.30	kJ/mol	NIST Webbook
log10ws	-2.69		Crippen Method
logp	2.822		Crippen Method
mcvol	169.960	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
tb	527.93	K	Joback Method
tc	741.38	K	Joback Method
tf	365.04	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.65	J/mol×K	527.93	Joback Method
cpg	458.37	J/mol×K	563.51	Joback Method
cpg	476.70	J/mol×K	599.08	Joback Method
cpg	493.91	J/mol×K	634.66	Joback Method
cpg	510.28	J/mol×K	670.23	Joback Method
cpg	526.10	J/mol×K	705.81	Joback Method
cpg	541.64	J/mol×K	741.38	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=C10395503&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume