

1-Methyl-2-norbornanone dimethyl ketal

Inchi: InChI=1S/C10H18O2/c1-9-5-4-8(6-9)7-10(9,11-2)12-3/h8H,4-7H2,1-3H3
InchiKey: AXBBFPXBQLLLSD-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: COC1(OC)CC2CCC1(C)C2
Mol. weight [g/mol]: 170.25
CAS: 26327-56-0

Physical Properties

Property code	Value	Unit	Source
gf	-85.97	kJ/mol	Joback Method
hf	-364.59	kJ/mol	Joback Method
hfus	6.68	kJ/mol	Joback Method
hvap	54.64 ± 0.08	kJ/mol	NIST Webbook
log10ws	-2.10		Crippen Method
logp	2.186		Crippen Method
mcvol	141.780	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
tb	486.60	K	Joback Method
tc	698.04	K	Joback Method
tf	322.84	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.81	J/mol×K	486.60	Joback Method
cpg	361.18	J/mol×K	521.84	Joback Method
cpg	378.17	J/mol×K	557.08	Joback Method
cpg	393.99	J/mol×K	592.32	Joback Method
cpg	408.83	J/mol×K	627.56	Joback Method
cpg	422.87	J/mol×K	662.80	Joback Method
cpg	436.31	J/mol×K	698.04	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26327560&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

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