

Muscone

Other names:	Cyclopentadecanone, 3-methyl- 3-Methylcyclopentadecanone 3-Methyl-1-cyclopentadecanone Moschus ketone Muskone Methylexaltone 3-methylcyclopentadecan-1-one
Inchi:	InChI=1S/C16H30O/c1-15-12-10-8-6-4-2-3-5-7-9-11-13-16(17)14-15/h15H,2-14H2,1H3
InchiKey:	ALHUZKCOMYUFRB-UHFFFAOYSA-N
Formula:	C16H30O
SMILES:	CC1CCCCCCCCCCCCC(=O)C1
Mol. weight [g/mol]:	238.41
CAS:	541-91-3

Physical Properties

Property code	Value	Unit	Source
gf	-123.20	kJ/mol	Joback Method
hf	-512.39	kJ/mol	Joback Method
hfus	9.64	kJ/mol	Joback Method
hvap	57.43	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	5.277		Crippen Method
mcvol	227.010	ml/mol	McGowan Method
pc	1908.57	kPa	Joback Method
rinpol	1831.00		NIST Webbook
ripol	2281.00		NIST Webbook
tb	691.28	K	Joback Method
tc	949.40	K	Joback Method
tf	314.00	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	683.83	J/mol×K	691.28	Joback Method
cpg	714.69	J/mol×K	734.30	Joback Method
cpg	742.99	J/mol×K	777.32	Joback Method
cpg	768.64	J/mol×K	820.34	Joback Method
cpg	791.53	J/mol×K	863.36	Joback Method
cpg	811.60	J/mol×K	906.38	Joback Method
cpg	828.73	J/mol×K	949.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C541913&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
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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