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]:	238.42

Physical Properties

Property code	Value	Unit	Source
af	0.3549		Cheméo Relay (1.0)
gf	-123.20	kJ/mol	Joback Method
hf	-495.12	kJ/mol	Cheméo Relay (1.0)
hfus	9.64	kJ/mol	Joback Method
hvap	73.27	kJ/mol	Cheméo Relay (1.0)
ie	9.00	eV	Cheméo Relay (1.0)
log10ws	-4.85		Cheméo Relay (1.0)
logp	5.277		Crippen Method
mcvol	227.010	ml/mol	McGowan Method
pc	1908.57	kPa	Joback Method
rinpol	1831.00		NIST Webbook
rinpol	1831.00		NIST Webbook
rinpol	1831.00		NIST Webbook
ripol	2281.00		NIST Webbook
ripol	2281.00		NIST Webbook
ripol	2281.00		NIST Webbook
tb	616.20	K	Cheméo Relay (1.0)
tc	823.30	K	Cheméo Relay (1.0)
tf	326.84	K	Cheméo Relay (1.0)
vc	0.727	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
hvapt	63.50	kJ/mol	496.00	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C541913&Units=SI

Legend

af: Acentric Factor
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
hvapt: Enthalpy of vaporization at a given temperature
ie: Ionization energy
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