Olean-12-en-28-oic acid, 3-oxo-, methyl ester

Other names:	Methyl oleanonate
	Methyl olean-12-en-3-oxo-28-oate
Inchi:	InChI=1S/C31H48O3/c1-26(2)15-17-31(25(33)34-8)18-16-29(6)20(21(31)19-26)9-10-23-
InchiKey:	PPMUFCXCVKVCSV-UHFFFAOYSA-N
Formula:	C31H48O3
SMILES:	COC(=O)C12CCC(C)(C)CC1C1=CCC3C4(C)CCC(=O)C(C)(C)C4CCC3(C)C1(C)CC2
Mol. weight [g/mol]:	468.71
CAS:	1721-58-0

Physical Properties

Property code	Value	Unit	Source
gf	29.23	kJ/mol	Joback Method
hf	-688.40	kJ/mol	Joback Method
hfus	21.65	kJ/mol	Joback Method
hvap	91.58	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	7.530		Crippen Method
mcvol	398.060	ml/mol	McGowan Method
pc	1021.38	kPa	Joback Method
rinpol	3512.00		NIST Webbook
rinpol	3512.00		NIST Webbook
tb	1103.28	K	Joback Method
tc	1368.22	K	Joback Method
tf	784.29	K	Joback Method
vc	1.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1730.08	J/mol×K	1103.28	Joback Method
cpg	1810.00	J/mol×K	1147.44	Joback Method
cpg	1899.07	J/mol×K	1191.59	Joback Method
cpg	1998.39	J/mol×K	1235.75	Joback Method
cpg	2109.06	J/mol×K	1279.91	Joback Method

cpg	2232.17	J/mol×K	1324.06	Joback Method
cpg	2368.81	J/mol×K	1368.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1721580&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume