Methyl palustrate

Other names:	1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,5,6,9,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, methyl ester, [1R-(1«alpha»,4a«beta»,10a«alpha»)]- Podocarpa-8,13-dien-15-oic acid, 13-isopropyl-, methyl ester Palastric acid, methyl ester
Inchi:	InChI=1S/C21H32O2/c1-14(2)15-7-9-17-16(13-15)8-10-18-20(17,3)11-6-12-21(18,4)19(2
InchiKey:	MEQSJWRGVQAVJY-MNLRITNHSA-N
Formula:	C21H32O2
SMILES:	COC(=O)C1(C)CCCC2(C)C3=C(C=C(C(C)C)CC3)CCC12
Mol. weight [g/mol]:	316.48
CAS:	3310-94-9

Physical Properties

Property code	Value	Unit	Source
gf	31.38	kJ/mol	Joback Method
hf	-427.62	kJ/mol	Joback Method
hfus	22.00	kJ/mol	Joback Method
hvap	71.97	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.439		Crippen Method
mcvol	273.010	ml/mol	McGowan Method
pc	1540.29	kPa	Joback Method
rinpol	2271.00		NIST Webbook
rinpol	2284.00		NIST Webbook
rinpol	2271.00		NIST Webbook
ripol	2876.00		NIST Webbook
ripol	2875.00		NIST Webbook
ripol	2875.00		NIST Webbook
tb	811.04	K	Joback Method
tc	1043.59	K	Joback Method
tf	506.69	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	883.85	J/mol×K	811.04	Joback Method
cpg	908.00	J/mol×K	849.80	Joback Method
cpg	931.89	J/mol×K	888.56	Joback Method
cpg	955.82	J/mol×K	927.31	Joback Method
cpg	980.09	J/mol×K	966.07	Joback Method
cpg	1004.99	J/mol×K	1004.83	Joback Method
cpg	1030.82	J/mol×K	1043.59	Joback Method

Sources

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=C3310949&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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