

1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,8a,9,10,10a-dodecahydro-1,4a-dimethyl ester

Other names: Podocarp-13-en-15-oic acid, 13-isopropyl-, methyl ester

[1R-(1«alpha»,4a«beta»,4b«alpha»,8a«beta»,10a«beta»)]-1,4a-dimethyl-1,2,3,4,4a,4b,5,6,8a,9,10,10a-dodecahydro-1H-phenanthrene-1-carboxylate

Inchi: InChI=1S/C21H34O2/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: MARRJGBPDCCA EK-UHFFFAOYSA-N

Formula: C21H34O2

SMILES: COC(=O)C1(C)CCCC2(C)C3CCC(C(C)C)=CC3CCC12

Mol. weight [g/mol]: 318.49

CAS: 33892-18-1

Physical Properties

Property code	Value	Unit	Source
gf	5.26	kJ/mol	Joback Method
hf	-503.14	kJ/mol	Joback Method
hfus	23.69	kJ/mol	Joback Method
hvap	69.74	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	5.375		Crippen Method
mcvol	277.310	ml/mol	McGowan Method
pc	1456.79	kPa	Joback Method
rinpol	2244.00		NIST Webbook
rinpol	2244.00		NIST Webbook
tb	792.58	K	Joback Method
tc	1022.06	K	Joback Method
tf	472.41	K	Joback Method
vc	1.040	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.37	J/molxK	792.58	Joback Method
cpg	942.05	J/molxK	830.83	Joback Method
cpg	967.14	J/molxK	869.07	Joback Method
cpg	991.94	J/molxK	907.32	Joback Method

cpg	1016.73	J/mol×K	945.56	Joback Method
cpg	1041.78	J/mol×K	983.81	Joback Method
cpg	1067.39	J/mol×K	1022.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33892181&Units=SI
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

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
hvp:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	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

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