1-Phenanthrenecarboxaldehyde, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-m [1R-(1«alpha»,4a«beta»,10a«alpha»)]-

Other names: (1R,4aS,10aR)-7-Isopropyl-1,4a-dimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthrene-1-
Podocarpa-8,11,13-trien-15-al, 13-isopropyl-
Dehydroabietal
Dehydroabietic aldehyde
Dehydroabietinal
Abietaldehyde, dehydro-

Inchi: InChI=1S/C20H28O/c1-14(2)15-6-8-17-16(12-15)7-9-18-19(3,13-21)10-5-11-20(17,18)4/

InchiKey: YCLCHPWRGSDZKL-IOJLRTSASA-N

Formula: C20H28O

SMILES: CC(C)c1ccc2c(c1)CCC1C(C)(C=O)CCCC21C

Mol. weight [g/mol]: 284.44

CAS: 13601-88-2

Physical Properties

Property code	Value	Unit	Source
gf	187.32	kJ/mol	Joback Method
hf	-189.98	kJ/mol	Joback Method
hfus	20.13	kJ/mol	Joback Method
hvap	67.61	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	5.019		Crippen Method
mcvol	248.750	ml/mol	McGowan Method
pc	1753.60	kPa	Joback Method
rinpol	2260.00		NIST Webbook
rinpol	2265.00		NIST Webbook
rinpol	2259.00		NIST Webbook
rinpol	2263.00		NIST Webbook
rinpol	2263.00		NIST Webbook
rinpol	2275.00		NIST Webbook
rinpol	2270.00		NIST Webbook
rinpol	2263.00		NIST Webbook
rinpol	2268.00		NIST Webbook
rinpol	2263.00		NIST Webbook
rinpol	2221.00		NIST Webbook
rinpol	2226.00		NIST Webbook
rinpol	2265.00		NIST Webbook
rinpol	2270.00		NIST Webbook

ripol	2981.00		NIST Webbook
ripol	2976.00		NIST Webbook
tb	759.69	K	Joback Method
tc	996.72	K	Joback Method
tf	466.02	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.98	J/mol×K	759.69	Joback Method
cpg	787.50	J/mol×K	799.19	Joback Method
cpg	809.58	J/mol×K	838.70	Joback Method
cpg	831.56	J/mol×K	878.20	Joback Method
cpg	853.76	J/mol×K	917.71	Joback Method
cpg	876.53	J/mol×K	957.21	Joback Method
cpg	900.19	J/mol×K	996.72	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=C13601882&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