Dehydroabietic acid

Other names:

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

(1R,4aS,10aR)-7-isopropyl-1,4a-dimethyl-1,2,3,4,4a,9,10,10a-octahydrophenanthrene-1-

Podocarpa-8,11,13-trien-15-oic acid, 13-isopropyl-

acid

Abieta-8,11,13-trien-18-oic acid

Abietic acid, dehydro-

Dehydroabietate

1,2,3,4,4a,9,10,10a-Octahydro-1,4a-dimethyl-7-(1-methylethyl)-1-phenanthrenecarboxylic

13-Isopropylpodocarpa-8,11,13-trien-15-oic acid

acid-, [1R-(1«alpha»,4a«beta»,10a«alpha»)]-

1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, (1R,4aS,10aR)-

NSC 2952

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

acid

Inchi: InChI=1S/C20H28O2/c1-13(2)14-6-8-16-15(12-14)7-9-17-19(16,3)10-5-11-20(17,4)18(21

InchiKey: NFWKVWVWBFBAOV-UUKMXZOPSA-N

Formula: C20H28O2

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

Mol. weight [g/mol]: 300.44

CAS: 1740-19-8

Physical Properties

Property code	Value	Unit	Source
gf	21.10	kJ/mol	Joback Method
hf	-369.21	kJ/mol	Joback Method
hfus	23.53	kJ/mol	Joback Method
hvap	84.31	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.905		Crippen Method
mcvol	254.620	ml/mol	McGowan Method
pc	1878.90	kPa	Joback Method
rinpol	2380.00		NIST Webbook
rinpol	399.90		NIST Webbook
rinpol	2457.00		NIST Webbook
tb	857.08	K	Joback Method
tc	1083.04	K	Joback Method
tf	534.77	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	836.11	J/mol×K	857.08	Joback Method
cpg	857.31	J/mol×K	894.74	Joback Method
cpg	878.82	J/mol×K	932.40	Joback Method
cpg	900.93	J/mol×K	970.06	Joback Method
cpg	923.92	J/mol×K	1007.72	Joback Method
cpg	948.09	J/mol×K	1045.38	Joback Method
cpg	973.73	J/mol×K	1083.04	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1740198&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
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
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