Abietic acid

Other names: (-)-Abietic acid

1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1«alpha»,4a«beta»,4b«alpha»,10a«alpha»)]-

1-Phenanthrenecarboxylic acid, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1Â«alphaÂ»,4aÂ«betaÂ»,4bÂ«alphaÂ»,10aÂ«alphaÂ»)]-

13-Isopropylpodocarpa-7,13-dien-15-oic acid

7,13-Abietadien-18-oic acid

Abietate

Abietinic acid

Kyselina abietova

L-abietic acid

NSC 25149

Podocarpa-7,13-dien-15-oic acid, 13-isopropyl-

Sylvic acid

Inchi: [1R-(1«alpha»,4a«beta»,4b«alpha»,10a«alpha»)]-1,2,3,4,4a,4b,5,6,10,10a-Decahydro-1,4a-dimethyl-7-(1-methylethyl)-1-phenanthrenecarboxylic acid

[1R-(1Â«alphaÂ»,4aÂ«betaÂ»,4bÂ«alphaÂ»,10aÂ«alphaÂ»)]-1,2,3,4,4a,4b,5,6,10,10a-Decahydro-1,4a-dimethyl-7-(1-methylethyl)-1-phenanthrenecarboxylic acid

InChI=1S/C20H30O2/c1-13(2)14-6-8-16-15(12-14)7-9-17-19(16,3)10-5-11-20(17,4)18(21)22/h12-13,16-17H,5-11H2,1-4H3,(H,21,22)/t16-,17-,19-,20-/m1/s1

InchiKey: RSWGJHLUYNHPMX-CSPVLLTOSA-N

Formula: C20H30O2

SMILES: CC(C)C1=CC2=CCC3C(C)(C(=O)O)CCCC3(C)C2CC1

Mol. weight [g/mol]: 302.45

CAS: 514-10-3

Physical Properties

Property code	Value	Unit	Source
gf	-6.94	kJ/mol	Joback Method
hf	-435.86	kJ/mol	Joback Method
hfus	19.45	kJ/mol	Measurement and correlation of solubility of abietic acid in ethanol + water mixtures
hvap	83.05	kJ/mol	Joback Method
log10ws	-3.80		Aqueous Solubility Prediction Method
logp	5.206		Crippen Method
mcvol	258.920	ml/mol	McGowan Method
pc	1793.94	kPa	Joback Method
rinpol	2512.70		NIST Webbook
tb	848.27	K	Joback Method
tc	1072.04	K	Joback Method

tf	446.65	K	Aqueous Solubility Prediction Method
tf	450.89	K	Measurement and correlation of solid-liquid equilibrium for abietic acid + alcohol systems at atmospheric pressure
vc	0.973	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	868.41	J/mol×K	848.27	Joback Method
cpg	890.49	J/mol×K	885.56	Joback Method
cpg	912.68	J/mol×K	922.86	Joback Method
cpg	935.26	J/mol×K	960.15	Joback Method
cpg	958.50	J/mol×K	997.45	Joback Method
cpg	982.69	J/mol×K	1034.74	Joback Method
cpg	1008.10	J/mol×K	1072.04	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37837e+01
Coeff. B	-4.12080e+03
Coeff. C	-2.07019e+02
Temperature range (K), min.	512.35
Temperature range (K), max.	693.41

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C514103&Units=SI

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Measurement and correlation of solid-liquid equilibrium for abietic acid + alcohol systems at atmospheric pressure:	https://www.doi.org/10.1016/j.fluid.2014.01.018
Measurement and correlation of solubility of abietic acid in ethanol + water mixtures:	https://www.doi.org/10.1016/j.jct.2013.07.015

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume