

Abieta-8,13(15)-dien-18-ol

Inchi:	InChI=1S/C20H32O/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:	IROXAKIPGBQTGG-AQNXPMDSA-N
Formula:	C20H32O
SMILES:	CC(C)=C1CCC2=C(CCC3C(C)(CO)CCCC23C)C1
Mol. weight [g/mol]:	288.47

Physical Properties

Property code	Value	Unit	Source
gf	139.08	kJ/mol	Joback Method
hf	-289.20	kJ/mol	Joback Method
hfus	22.41	kJ/mol	Joback Method
hvap	77.57	kJ/mol	Joback Method
log10ws	-6.12		Crippen Method
logp	5.402		Crippen Method
mcvol	257.350	ml/mol	McGowan Method
pc	1734.67	kPa	Joback Method
rinpol	2271.00		NIST Webbook
rinpol	2271.00		NIST Webbook
tb	806.87	K	Joback Method
tc	1027.65	K	Joback Method
tf	482.20	K	Joback Method
vc	0.972	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.08	J/mol×K	806.87	Joback Method
cpg	863.50	J/mol×K	843.67	Joback Method
cpg	885.81	J/mol×K	880.46	Joback Method
cpg	908.29	J/mol×K	917.26	Joback Method
cpg	931.24	J/mol×K	954.06	Joback Method
cpg	954.92	J/mol×K	990.86	Joback Method
cpg	979.62	J/mol×K	1027.65	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R576479&Units=SI

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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