

Abieta-8(14),13(15)-diene

Inchi:	InChI=1S/C20H32/c1-14(2)15-7-9-17-16(13-15)8-10-18-19(3,4)11-6-12-20(17,18)5/h13,1
InchiKey:	MRRHSEMHYVQUFK-UHFFFAOYSA-N
Formula:	C20H32
SMILES:	CC(C)=C1C=C2CCC3C(C)(C)CCCC3(C)C2CC1
Mol. weight [g/mol]:	272.47

Physical Properties

Property code	Value	Unit	Source
gf	277.82	kJ/mol	Joback Method
hf	-145.84	kJ/mol	Joback Method
hfus	19.78	kJ/mol	Joback Method
hvap	59.92	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	6.286		Crippen Method
mcvol	251.480	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	2154.00		NIST Webbook
rinpol	2147.00		NIST Webbook
rinpol	2150.00		NIST Webbook
rinpol	2121.00		NIST Webbook
rinpol	2154.00		NIST Webbook
rinpol	2147.00		NIST Webbook
tb	705.04	K	Joback Method
tc	941.51	K	Joback Method
tf	404.62	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.59	J/molxK	705.04	Joback Method
cpg	792.65	J/molxK	744.45	Joback Method
cpg	817.69	J/molxK	783.86	Joback Method
cpg	842.05	J/molxK	823.27	Joback Method

cpg	866.08	J/mol×K	862.68	Joback Method
cpg	890.10	J/mol×K	902.10	Joback Method
cpg	914.46	J/mol×K	941.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R287926&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

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
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

Latest version available from:

<https://www.chemeo.com/cid/21-952-1/Abieta-8-14-13-15-diene.pdf>

Generated by Cheméo on 2024-04-25 06:15:36.970202075 +0000 UTC m=+16314985.890779397.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.