Abieta-8,12-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/h7,14
InchiKey: BGVUIJDZTQIJIO-IJHRGXPZSA-N
Formula: C20H32
SMILES: CC(C)C1=CCC2=C(CCC3C(C)(C)CCCC23C)C1
Mol. weight [g/mol]: 272.47

Physical Properties

Property code	Value	Unit	Source
gf	256.88	kJ/mol	Joback Method
hf	-162.18	kJ/mol	Joback Method
hfus	16.62	kJ/mol	Joback Method
hvap	60.59	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	6.286		Crippen Method
mcvol	251.480	ml/mol	McGowan Method
pc	1602.56	kPa	Joback Method
rinpol	1983.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	2023.00		NIST Webbook
rinpol	2022.00		NIST Webbook
rinpol	2011.00		NIST Webbook
rinpol	1983.00		NIST Webbook
rinpol	2023.00		NIST Webbook
tb	711.87	K	Joback Method
tc	946.21	K	Joback Method
tf	423.26	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.74	J/mol×K	711.87	Joback Method
cpg	789.91	J/mol×K	750.93	Joback Method
cpg	814.18	J/mol×K	789.98	Joback Method

cpg	837.86	J/mol×K	829.04	Joback Method
cpg	861.28	J/mol×K	868.09	Joback Method
cpg	884.76	J/mol×K	907.15	Joback Method
cpg	908.63	J/mol×K	946.21	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R301978&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
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