Abieta-7,11-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/h7-9,
InchiKey: KJYQZJWXFQWVEO-ZMXXURFWSA-N
Formula: C20H32
SMILES: CC(C)C1C=CC2C(=CCC3C(C)(C)CCCC23C)C1
Mol. weight [g/mol]: 272.47

Physical Properties

Property code	Value	Unit	Source
gf	260.72	kJ/mol	Joback Method
hf	-179.92	kJ/mol	Joback Method
hfus	19.54	kJ/mol	Joback Method
hvap	58.65	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	5.997		Crippen Method
mcvol	251.480	ml/mol	McGowan Method
pc	1557.35	kPa	Joback Method
rinpol	2043.00		NIST Webbook
rinpol	2067.00		NIST Webbook
rinpol	2017.00		NIST Webbook
tb	692.57	K	Joback Method
tc	925.50	K	Joback Method
tf	389.74	K	Joback Method
vc	0.947	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.50	J/mol×K	692.57	Joback Method
cpg	793.97	J/mol×K	731.39	Joback Method
cpg	819.28	J/mol×K	770.21	Joback Method
cpg	843.73	J/mol×K	809.04	Joback Method
cpg	867.63	J/mol×K	847.86	Joback Method
cpg	891.32	J/mol×K	886.68	Joback Method
cpg	915.09	J/mol×K	925.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R387125&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

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