Abienol

Inchi: InChI=1S/C20H34O/c1-7-15(2)9-10-17-19(5)13-8-12-18(3,4)16(19)11-14-20(17,6)21/h7,9

InchiKey: ZAZVCYBIABTSJR-HFTPNAHGSA-N

Formula: C20H34O

SMILES: C=CC(C)=CCC1C(C)(O)CCC2C(C)(C)CCCC21C

Mol. weight [g/mol]: 290.48

Physical Properties

Property code	Value	Unit	Source
hfus	21.45	kJ/mol	Joback Method
logp	5.502		Crippen Method
mcvol	268.210	ml/mol	McGowan Method
rinpol	2103.00		NIST Webbook
rinpol	2103.00		NIST Webbook
ripol	2626.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	856.65	J/mol×K	767.17	Joback Method
cpg	880.12	J/mol×K	802.55	Joback Method
cpg	903.54	J/mol×K	837.94	Joback Method
cpg	927.22	J/mol×K	873.32	Joback Method
cpg	951.49	J/mol×K	908.71	Joback Method
cpg	976.65	J/mol×K	944.09	Joback Method
cpg	1003.03	J/mol×K	979.48	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R291346&Units=SI

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

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices