

phyllocladanol

Inchi:	InChI=1S/C20H34O/c1-17(2)9-5-10-18(3)15(17)8-11-20-12-14(6-7-16(18)20)19(4,21)13-
InchiKey:	FZSRMADKTOBCNT-UHFFFAOYSA-N
Formula:	C20H34O
SMILES:	CC1(C)CCC[C@@]2(C)C1CC[C@@]13C[C@@H](CCC12)[C@](C)(O)C3
Mol. weight [g/mol]:	290.49

Physical Properties

Property code	Value	Unit	Source
hfus	13.80	kJ/mol	Joback Method
logp	5.170		Crippen Method
mcpvol	255.090	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	873.24	J/mol×K	780.17	Joback Method
cpg	899.87	J/mol×K	818.29	Joback Method
cpg	927.16	J/mol×K	856.41	Joback Method
cpg	955.65	J/mol×K	894.53	Joback Method
cpg	985.88	J/mol×K	932.65	Joback Method
cpg	1018.38	J/mol×K	970.77	Joback Method
cpg	1053.70	J/mol×K	1008.89	Joback Method

Sources

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.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R167263&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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