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-BEMISUSKSA-N
Formula: C20H34O
SMILES: CC1(C)CCCC2(C)C1CCC13CC(CCC12)C(C)(O)C3
Mol. weight [g/mol]: 290.48

Physical Properties

Property code	Value	Unit	Source
hfus	13.80	kJ/mol	Joback Method
logp	5.170		Crippen Method
mcvol	255.090	ml/mol	McGowan Method
rinpol	2210.00		NIST Webbook
rinpol	2200.00		NIST Webbook
rinpol	2200.00		NIST Webbook
rinpol	2210.00		NIST Webbook
rinpol	2210.00		NIST Webbook
rinpol	2200.00		NIST Webbook
rinpol	2205.00		NIST Webbook
rinpol	2180.00		NIST Webbook
ripol	2835.00		NIST Webbook
ripol	2865.00		NIST Webbook

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R167263&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