Decalin-6«beta»-pentanoic acid, «gamma»,1,1,5«beta»,7«alpha»-pentamethyl, methyl ester, #1

Inchi: InChI=1S/C20H36O2/c1-13(9-10-18(21)22-6)19-14(2)12-17-16(15(19)3)8-7-11-20(17,4)5

InchiKey: ANIOXIWWKFCWCF-VIHNPHLRSA-N

Formula: C20H36O2

SMILES: COC(=O)CCC(C)C1C(C)CC2C(CCCC2(C)C)C1C

Mol. weight [g/mol]: 308.50

Physical Properties

Property code	Value	Unit	Source
hfus	32.68	kJ/mol	Joback Method
logp	5.310		Crippen Method
mcvol	278.380	ml/mol	McGowan Method
rinpol	1995.00		NIST Webbook
rinpol	1995.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	900.20	J/mol×K	744.97	Joback Method
cpg	924.96	J/mol×K	779.37	Joback Method
cpg	948.52	J/mol×K	813.77	Joback Method
cpg	970.99	J/mol×K	848.16	Joback Method
cpg	992.47	J/mol×K	882.56	Joback Method
cpg	1013.06	J/mol×K	916.96	Joback Method
cpg	1032.87	J/mol×K	951.36	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R554053&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

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