Kolavelool (2 epimers)

Inchi: InChI=1S/C21H36O/c1-16(12-15-22-6)10-13-20(4)18(3)11-14-21(5)17(2)8-7-9-19(20)21/
InchiKey: YAJBRZZIZBUICV-COIMSNGRSA-N
Formula: C21H36O
SMILES: COCC=C(C)CCC1(C)C(C)CCC2(C)C(C)=CCCC21
Mol. weight [g/mol]: 304.51

Physical Properties

Property code	Value	Unit	Source
gf	159.64	kJ/mol	Joback Method
hf	-344.49	kJ/mol	Joback Method
hfus	28.47	kJ/mol	Joback Method
hvap	63.34	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	6.158		Crippen Method
mcvol	282.300	ml/mol	McGowan Method
pc	1285.59	kPa	Joback Method
rinpol	2050.00		NIST Webbook
tb	732.18	K	Joback Method
tc	944.77	K	Joback Method
tf	404.02	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.61	J/mol×K	732.18	Joback Method
cpg	896.49	J/mol×K	767.61	Joback Method
cpg	920.60	J/mol×K	803.04	Joback Method
cpg	944.15	J/mol×K	838.47	Joback Method
cpg	967.36	J/mol×K	873.90	Joback Method
cpg	990.47	J/mol×K	909.33	Joback Method
cpg	1013.68	J/mol×K	944.77	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R227093&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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