

Trachylobanic acid, methyl ester

Inchi: InChI=1S/C21H32O2/c1-18-7-5-8-19(2,17(22)23-4)15(18)6-9-21-11-14-13(10-16(18)21)2
InchiKey: DBYBRADCKQFKPC-SGLDGZOLSA-N
Formula: C21H32O2
SMILES: COC(=O)C1(C)CCCC2(C)C3CC4C5CC3(CCC12)CC45C
Mol. weight [g/mol]: 316.48

Physical Properties

Property code	Value	Unit	Source
gf	138.58	kJ/mol	Joback Method
hf	-363.79	kJ/mol	Joback Method
hfus	19.53	kJ/mol	Joback Method
hvap	65.70	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.818		Crippen Method
mcvol	259.890	ml/mol	McGowan Method
pc	1690.72	kPa	Joback Method
rinpol	2278.00		NIST Webbook
rinpol	2278.00		NIST Webbook
tb	781.09	K	Joback Method
tc	1019.88	K	Joback Method
tf	567.65	K	Joback Method
vc	1.002	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	888.29	J/mol×K	781.09	Joback Method
cpg	915.64	J/mol×K	820.89	Joback Method
cpg	943.94	J/mol×K	860.69	Joback Method
cpg	973.85	J/mol×K	900.48	Joback Method
cpg	1006.03	J/mol×K	940.28	Joback Method
cpg	1041.14	J/mol×K	980.08	Joback Method
cpg	1079.84	J/mol×K	1019.88	Joback Method

Sources

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=R559187&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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