Methyl 7-isopropyl-1,4a-dimethyltetradecahydrophenantl

Inchi: InChI=1S/C21H36O2/c1-14(2)15-7-9-17-16(13-15)8-10-18-20(17,3)11-6-12-21(18,4)19(2

InchiKey: FJHHBOWEISXQJX-UHFFFAOYSA-N

Formula: C21H36O2

SMILES: COC(=O)C1(C)CCCC2(C)C3CCC(C(C)C)CC3CCC12

Mol. weight [g/mol]: 320.51

CAS: 32208-29-0

Physical Properties

Property code	Value	Unit	Source
gf	-22.78	kJ/mol	Joback Method
hf	-569.79	kJ/mol	Joback Method
hfus	23.93	kJ/mol	Joback Method
hvap	68.48	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	5.454		Crippen Method
mcvol	281.610	ml/mol	McGowan Method
pc	1398.55	kPa	Joback Method
rinpol	2308.50		NIST Webbook
rinpol	2308.50		NIST Webbook
tb	783.77	K	Joback Method
tc	1010.86	K	Joback Method
tf	454.89	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.39	J/mol×K	783.77	Joback Method
cpg	972.31	J/mol×K	821.62	Joback Method
cpg	998.47	J/mol×K	859.47	Joback Method
cpg	1024.15	J/mol×K	897.31	Joback Method
cpg	1049.62	J/mol×K	935.16	Joback Method
cpg	1075.15	J/mol×K	973.01	Joback Method
cpg	1101.01	J/mol×K	1010.86	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C32208290&Units=SI

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