(1R,4aS,10aR)-7-Isopropyl-1,4a-dimethyl-1,2,3,4,4

Other names: Palustral
Palustrinal
Inchi: InChI=1S/C20H30O/c1-14(2)15-6-8-17-16(12-15)7-9-18-19(3,13-21)10-5-11-20(17,18)4/
InchiKey: MDWQSNIQXHNTCK-UHFFFAOYSA-N
Formula: C20H30O
SMILES: CC(C)C1=CC2=C(CC1)C1(C)CCCC(C)(C=O)C1CC2
Mol. weight [g/mol]: 286.45
CAS: 13508-03-7

Physical Properties

Property code	Value	Unit	Source
gf	157.36	kJ/mol	Joback Method
hf	-247.76	kJ/mol	Joback Method
hfus	18.91	kJ/mol	Joback Method
hvap	67.31	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.465		Crippen Method
mcvol	253.050	ml/mol	McGowan Method
pc	1701.90	kPa	Joback Method
rinpol	2245.20		NIST Webbook
rinpol	2204.00		NIST Webbook
rinpol	2200.00		NIST Webbook
rinpol	2204.00		NIST Webbook
ripol	2854.00		NIST Webbook
ripol	2845.00		NIST Webbook
tb	760.53	K	Joback Method
tc	995.64	K	Joback Method
tf	465.26	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.07	J/mol×K	760.53	Joback Method

cpg	814.51	J/mol×K	799.72	Joback Method
cpg	837.46	J/mol×K	838.90	Joback Method
cpg	860.23	J/mol×K	878.09	Joback Method
cpg	883.15	J/mol×K	917.27	Joback Method
cpg	906.55	J/mol×K	956.46	Joback Method
cpg	930.75	J/mol×K	995.64	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=C13508037&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume