((1S,4aR,4bR,10aR)-7-Isopropyl-1,4a-dimethyl-1,2,

Inchi: InChI=1S/C20H32O/c1-14(2)15-6-8-17-16(12-15)7-9-18-19(3,13-21)10-5-11-20(17,18)4/h
InchiKey: GQRUHVMVWNKUFW-UHFFFAOYSA-N
Formula: C20H32O
SMILES: CC(C)C1=CC2=CCC3C(C)(CO)CCCC3(C)C2CC1
Mol. weight [g/mol]: 288.47
CAS: 24563-94-8

Physical Properties

Property code	Value	Unit	Source
gf	121.98	kJ/mol	Joback Method
hf	-323.28	kJ/mol	Joback Method
hfus	22.17	kJ/mol	Joback Method
hvap	76.30	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	5.114		Crippen Method
mcvol	257.350	ml/mol	McGowan Method
pc	1701.90	kPa	Joback Method
rinpol	2340.00		NIST Webbook
rinpol	2374.90		NIST Webbook
rinpol	2374.90		NIST Webbook
tb	794.40	K	Joback Method
tc	1012.23	K	Joback Method
tf	467.32	K	Joback Method
vc	0.967	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.75	J/mol×K	794.40	Joback Method
cpg	866.15	J/mol×K	830.71	Joback Method
cpg	888.26	J/mol×K	867.01	Joback Method
cpg	910.36	J/mol×K	903.32	Joback Method
cpg	932.70	J/mol×K	939.62	Joback Method
cpg	955.55	J/mol×K	975.93	Joback Method

cpg	979.16	J/mol×K	1012.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24563948&Units=SI
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

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