(1R,4aR,4bS,10aR)-1,4a-Dimethyl-7-(propan-2-ylid

Other names: Neoabietal
Neoabietinal
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: JPCTZWFFRZZTMM-UHFFFAOYSA-N
Formula: C20H30O
SMILES: CC(C)=C1C=C2CCC3C(C)(C=O)CCCC3(C)C2CC1
Mol. weight [g/mol]: 286.45
CAS: 19898-57-8

Physical Properties

Property code	Value	Unit	Source
gf	178.30	kJ/mol	Joback Method
hf	-231.42	kJ/mol	Joback Method
hfus	22.07	kJ/mol	Joback Method
hvap	66.64	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.465		Crippen Method
mcvol	253.050	ml/mol	McGowan Method
pc	1683.79	kPa	Joback Method
rinpol	2321.00		NIST Webbook
tb	753.70	K	Joback Method
tc	990.82	K	Joback Method
tf	446.62	K	Joback Method
vc	0.969	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.85	J/mol×K	753.70	Joback Method
cpg	818.04	J/mol×K	793.22	Joback Method
cpg	841.63	J/mol×K	832.74	Joback Method
cpg	864.97	J/mol×K	872.26	Joback Method
cpg	888.40	J/mol×K	911.78	Joback Method
cpg	912.26	J/mol×K	951.30	Joback Method

cpg	936.89	J/mol×K	990.82	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=C19898578&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume