neoabietinol

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: MUBMRBNHMHINMF-UHFFFAOYSA-N
Formula: C20H32O
SMILES: CC(C)=C1C=C2CCC3C(C)(CO)CCCC3(C)C2CC1
Mol. weight [g/mol]: 288.47
CAS: 640-42-6

Physical Properties

Property code	Value	Unit	Source
gf	141.00	kJ/mol	Joback Method
hf	-298.07	kJ/mol	Joback Method
hfus	23.87	kJ/mol	Joback Method
hvap	76.60	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	5.258		Crippen Method
mcvol	257.350	ml/mol	McGowan Method
pc	1708.95	kPa	Joback Method
rinpol	2455.00		NIST Webbook
rinpol	2504.90		NIST Webbook
rinpol	2400.00		NIST Webbook
rinpol	2406.00		NIST Webbook
rinpol	2504.90		NIST Webbook
tb	797.22	K	Joback Method
tc	1017.18	K	Joback Method
tf	465.44	K	Joback Method
vc	0.971	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	844.03	J/mol×K	797.22	Joback Method
cpg	866.71	J/mol×K	833.88	Joback Method
cpg	889.15	J/mol×K	870.54	Joback Method
cpg	911.64	J/mol×K	907.20	Joback Method

cpg	934.46	J/mol×K	943.86	Joback Method
cpg	957.87	J/mol×K	980.52	Joback Method
cpg	982.16	J/mol×K	1017.18	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=C640426&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