13-Isopropylpodocarpen-12-ol-20-al

Inchi: InChI=1S/C20H28O2/c1-13(2)15-10-14-6-7-18-19(3,4)8-5-9-20(18,12-21)16(14)11-17(15
InchiKey: YPWYNONCSGZEQQ-UHFFFAOYSA-N
Formula: C20H28O2
SMILES: CC(C)c1cc2c(cc1O)C1(C=O)CCCC(C)(C)C1CC2
Mol. weight [g/mol]: 300.44
CAS: 24035-37-8

Physical Properties

Property code	Value	Unit	Source
gf	32.70	kJ/mol	Joback Method
hf	-367.29	kJ/mol	Joback Method
hfus	25.91	kJ/mol	Joback Method
hvap	80.62	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.725		Crippen Method
mcvol	254.620	ml/mol	McGowan Method
pc	1994.77	kPa	Joback Method
rinpol	2502.00		NIST Webbook
rinpol	2568.50		NIST Webbook
rinpol	2502.00		NIST Webbook
rinpol	2568.50		NIST Webbook
rinpol	2502.00		NIST Webbook
tb	840.31	K	Joback Method
tc	1083.78	K	Joback Method
tf	577.74	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	829.42	J/mol×K	840.31	Joback Method
cpg	852.37	J/mol×K	880.89	Joback Method
cpg	875.90	J/mol×K	921.47	Joback Method
cpg	900.42	J/mol×K	962.04	Joback Method

cpg	926.36	J/mol×K	1002.62	Joback Method
cpg	954.12	J/mol×K	1043.20	Joback Method
cpg	984.14	J/mol×K	1083.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24035378&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

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