Jaeschkeanin

Inchi: InChI=1S/C22H30O5/c1-13(2)22(25)10-9-20(3)12-17-21(4,27-17)11-16(18(20)22)26-19(
InchiKey: NZRACXOBLXBSFK-ORHJNQCKSA-N
Formula: C22H30O5
SMILES: CC(C)C1(O)CCC2(C)CC3OC3(C)CC(OC(=O)c3ccc(O)cc3)C21
Mol. weight [g/mol]: 374.47

Physical Properties

Property code	Value	Unit	Source
gf	-248.70	kJ/mol	Joback Method
hf	-781.72	kJ/mol	Joback Method
hfus	38.41	kJ/mol	Joback Method
hvap	105.52	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.672		Crippen Method
mcvol	289.550	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	2826.00		NIST Webbook
rinpol	2826.00		NIST Webbook
tb	1020.51	K	Joback Method
tc	1263.77	K	Joback Method
tf	726.15	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1106.50	J/mol×K	1020.51	Joback Method
cpg	1143.02	J/mol×K	1061.05	Joback Method
cpg	1183.10	J/mol×K	1101.60	Joback Method
cpg	1227.32	J/mol×K	1142.14	Joback Method
cpg	1276.21	J/mol×K	1182.68	Joback Method
cpg	1330.35	J/mol×K	1223.23	Joback Method
cpg	1390.28	J/mol×K	1263.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R200281&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