Panduratin A

Inchi: InChI=1S/C26H30O4/c1-16(2)10-12-20-17(3)11-13-21(18-8-6-5-7-9-18)24(20)26(29)25-2
InchiKey: LYDZCXVWCFJAKQ-UHFFFAOYSA-N
Formula: C26H30O4
SMILES: COc1cc(O)c(C(=O)C2C(CC=C(C)C)C(C)=CCC2c2ccccc2)c(O)c1
Mol. weight [g/mol]: 406.51
CAS: 89837-52-5

Physical Properties

Property code	Value	Unit	Source
gf	-58.90	kJ/mol	Joback Method
hf	-550.42	kJ/mol	Joback Method
hfus	58.84	kJ/mol	Joback Method
hvap	114.67	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	6.012		Crippen Method
mcvol	329.400	ml/mol	McGowan Method
pc	1592.35	kPa	Joback Method
rinpol	3191.10		NIST Webbook
rinpol	3191.10		NIST Webbook
tb	1108.54	K	Joback Method
tc	1368.37	K	Joback Method
tf	736.88	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1156.54	J/mol×K	1108.54	Joback Method
cpg	1176.07	J/mol×K	1151.85	Joback Method
cpg	1195.63	J/mol×K	1195.15	Joback Method
cpg	1215.48	J/mol×K	1238.46	Joback Method
cpg	1235.88	J/mol×K	1281.76	Joback Method
cpg	1257.05	J/mol×K	1325.07	Joback Method
cpg	1279.26	J/mol×K	1368.37	Joback Method

Sources

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=C89837525&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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