Nicolaioidesin C

Inchi: InChI=1S/C26H30O4/c1-17(2)8-7-9-18-12-13-21(22(14-18)19-10-5-4-6-11-19)26(29)25-2
InchiKey: VJYZXZFPGQYBKT-UHFFFAOYSA-N
Formula: C26H30O4
SMILES: COc1cc(O)c(C(=O)C2CC=C(CCC=C(C)C)CC2c2ccccc2)c(O)c1
Mol. weight [g/mol]: 406.51
CAS: 475579-27-2

Physical Properties

Property code	Value	Unit	Source
gf	-51.19	kJ/mol	Joback Method
hf	-530.08	kJ/mol	Joback Method
hfus	57.77	kJ/mol	Joback Method
hvap	114.98	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	6.156		Crippen Method
mcvol	329.400	ml/mol	McGowan Method
pc	1635.13	kPa	Joback Method
rinpol	3225.30		NIST Webbook
rinpol	3225.30		NIST Webbook
tb	1113.21	K	Joback Method
tc	1373.43	K	Joback Method
tf	741.12	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1152.44	J/mol×K	1113.21	Joback Method
cpg	1172.41	J/mol×K	1156.58	Joback Method
cpg	1192.60	J/mol×K	1199.95	Joback Method
cpg	1213.29	J/mol×K	1243.32	Joback Method
cpg	1234.73	J/mol×K	1286.69	Joback Method
cpg	1257.18	J/mol×K	1330.06	Joback Method
cpg	1280.92	J/mol×K	1373.43	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=C475579272&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