«gamma»-Ponalactone

Inchi: InChI=1S/C19H22O6/c1-7(2)12-8-5-10-14-18(3,9(8)6-11(20)24-12)16-13(25-16)15(21)19

InchiKey: KDORDIOOUCRJPK-TUGODLKSSA-N

Formula: C19H22O6

SMILES: CC(C)C1OC(=O)C=C2C1=CC1OC(=O)C3(C)C(O)C4OC4C2(C)C13

Mol. weight [g/mol]: 346.37

Physical Properties

Property code	Value	Unit	Source
gf	-247.60	kJ/mol	Joback Method
hf	-850.64	kJ/mol	Joback Method
hfus	47.25	kJ/mol	Joback Method
hvap	94.79	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	1.130		Crippen Method
mcvol	242.290	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
ripol	2029.00		NIST Webbook
tb	979.34	K	Joback Method
tc	1221.54	K	Joback Method
tf	710.16	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	931.02	J/mol×K	979.34	Joback Method
cpg	956.27	J/mol×K	1019.71	Joback Method
cpg	982.90	J/mol×K	1060.07	Joback Method
cpg	1011.28	J/mol×K	1100.44	Joback Method
cpg	1041.74	J/mol×K	1140.81	Joback Method
cpg	1074.63	J/mol×K	1181.17	Joback Method
cpg	1110.31	J/mol×K	1221.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R337165&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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