

GA120-isolactone, Me

Inchi:	InChI=1S/C20H24O4/c1-11-9-19-10-12(11)5-6-13(19)20-8-4-7-18(2,17(22)24-20)15(20)1
InchiKey:	QDGNFHLTCPXSCV-XNFUDPCWSA-N
Formula:	C20H24O4
SMILES:	<chem>C=C1CC23CC1CCC2C12C=CCC(C)(C(=O)O1)C2C3C(=O)OC</chem>
Mol. weight [g/mol]:	328.40

Physical Properties

Property code	Value	Unit	Source
gf	5.59	kJ/mol	Joback Method
hf	-471.89	kJ/mol	Joback Method
hfus	27.62	kJ/mol	Joback Method
hvap	74.32	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.030		Crippen Method
mcvol	244.640	ml/mol	McGowan Method
pc	1989.43	kPa	Joback Method
rinpol	2378.00		NIST Webbook
rinpol	2378.00		NIST Webbook
rinpol	2427.00		NIST Webbook
rinpol	2428.00		NIST Webbook
tb	860.00	K	Joback Method
tc	1111.71	K	Joback Method
tf	642.43	K	Joback Method
vc	0.939	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	856.88	J/molxK	860.00	Joback Method
cpg	883.23	J/molxK	901.95	Joback Method
cpg	911.08	J/molxK	943.90	Joback Method
cpg	941.00	J/molxK	985.85	Joback Method
cpg	973.57	J/molxK	1027.81	Joback Method
cpg	1009.34	J/molxK	1069.76	Joback Method

Sources

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=R281042&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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