(E)-Labda-8(17),12-diene-15,16-dial

Inchi: InChI=1S/C20H30O2/c1-15-6-9-18-19(2,3)11-5-12-20(18,4)17(15)8-7-16(14-22)10-13-21
InchiKey: TZCSIFOYBLPUIF-FRKPEAEDSA-N
Formula: C20H30O2
SMILES: C=C1CCC2C(C)(C)CCCC2(C)C1CC=C(C=O)CC=O
Mol. weight [g/mol]: 302.45
CAS: 104263-85-6

Physical Properties

Property code	Value	Unit	Source
gf	89.93	kJ/mol	Joback Method
hf	-324.86	kJ/mol	Joback Method
hfus	27.28	kJ/mol	Joback Method
hvap	71.34	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.890		Crippen Method
mcvol	265.480	ml/mol	McGowan Method
pc	1562.28	kPa	Joback Method
rinpol	2382.80		NIST Webbook
rinpol	2382.80		NIST Webbook
tb	779.22	K	Joback Method
tc	999.86	K	Joback Method
tf	454.92	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	832.90	J/mol×K	779.22	Joback Method
cpg	854.95	J/mol×K	815.99	Joback Method
cpg	876.60	J/mol×K	852.77	Joback Method
cpg	898.11	J/mol×K	889.54	Joback Method
cpg	919.75	J/mol×K	926.32	Joback Method
cpg	941.77	J/mol×K	963.09	Joback Method
cpg	964.43	J/mol×K	999.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104263856&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

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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