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

Inchi: InChI=1S/C19H28O2/c1-14-6-9-17-18(2,3)10-5-11-19(17,4)16(14)8-7-15(12-20)13-21/h7
InchiKey: HFTMAWAUKKDXCR-LVLJQFTKSA-N
Formula: C19H28O2
SMILES: C=C1CCC2C(C)(C)CCCC2(C)C1CC=C(C=O)C=O
Mol. weight [g/mol]: 288.42

Physical Properties

Property code	Value	Unit	Source
gf	81.51	kJ/mol	Joback Method
hf	-304.22	kJ/mol	Joback Method
hfus	24.69	kJ/mol	Joback Method
hvap	69.12	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.500		Crippen Method
mcvol	251.390	ml/mol	McGowan Method
pc	1687.95	kPa	Joback Method
rinpol	2220.00		NIST Webbook
rinpol	2220.00		NIST Webbook
ripol	2900.00		NIST Webbook
tb	756.34	K	Joback Method
tc	980.16	K	Joback Method
tf	443.65	K	Joback Method
vc	0.975	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	773.91	J/mol×K	756.34	Joback Method
cpg	795.44	J/mol×K	793.64	Joback Method
cpg	816.48	J/mol×K	830.95	Joback Method
cpg	837.30	J/mol×K	868.25	Joback Method
cpg	858.16	J/mol×K	905.55	Joback Method
cpg	879.32	J/mol×K	942.86	Joback Method
cpg	901.04	J/mol×K	980.16	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=R224529&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume