2-Hydroxyguia-1(10),11-dien-15-oic acid

Inchi: InChI=1S/C15H22O3/c1-8(2)10-4-5-11(15(17)18)14-12(7-10)9(3)6-13(14)16/h9-10,12-13
InchiKey: RKFHUZKKJPEXJC-UHFFFAOYSA-N
Formula: C15H22O3
SMILES: C=C(C)C1CCC(C(=O)O)=C2C(O)CC(C)C2C1
Mol. weight [g/mol]: 250.33

Physical Properties

Property code	Value	Unit	Source
gf	-179.47	kJ/mol	Joback Method
hf	-539.21	kJ/mol	Joback Method
hfus	32.25	kJ/mol	Joback Method
hvap	90.01	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	2.761		Crippen Method
mcvol	205.200	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinpol	1932.00		NIST Webbook
rinpol	1934.00		NIST Webbook
rinpol	1934.00		NIST Webbook
rinpol	1932.00		NIST Webbook
tb	807.73	K	Joback Method
tc	1009.03	K	Joback Method
tf	453.78	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.38	J/mol×K	807.73	Joback Method
cpg	677.68	J/mol×K	841.28	Joback Method
cpg	691.05	J/mol×K	874.83	Joback Method
cpg	703.52	J/mol×K	908.38	Joback Method
cpg	715.13	J/mol×K	941.93	Joback Method
cpg	725.91	J/mol×K	975.48	Joback Method

cpg	735.92	J/mol×K	1009.03	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=R612941&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