(4«beta»)-kaur-16-en-18-oic acid

Inchi: InChI=1S/C20H30O2/c1-13-11-20-10-7-15-18(2,16(20)6-5-14(13)12-20)8-4-9-19(15,3)17
InchiKey: NIKHGUQULKYIGE-UKIWHTGDSA-N
Formula: C20H30O2
SMILES: C=C1CC23CCC4C(C)(C(=O)O)CCCC4(C)C2CCC1C3
Mol. weight [g/mol]: 302.45

Physical Properties

Property code	Value	Unit	Source
gf	67.57	kJ/mol	Joback Method
hf	-365.10	kJ/mol	Joback Method
hfus	19.47	kJ/mol	Joback Method
hvap	79.97	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	5.040		Crippen Method
mcvol	252.360	ml/mol	McGowan Method
pc	1932.13	kPa	Joback Method
rinpol	2358.00		NIST Webbook
rinpol	2358.00		NIST Webbook
tb	837.63	K	Joback Method
tc	1066.59	K	Joback Method
tf	560.49	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	874.87	J/mol×K	837.63	Joback Method
cpg	899.64	J/mol×K	875.79	Joback Method
cpg	925.24	J/mol×K	913.95	Joback Method
cpg	952.11	J/mol×K	952.11	Joback Method
cpg	980.69	J/mol×K	990.27	Joback Method
cpg	1011.41	J/mol×K	1028.43	Joback Method
cpg	1044.72	J/mol×K	1066.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R289299&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume