Kaur-16-en-18-oic acid, methyl ester, (4«beta»)-

Other names: Kaur-16-en-19-oic acid, methyl ester
Argyrophilic acid methyl ester
Methyl kaur-16-en-18-oate, ((4«beta»)-
ent-Kaurenoic acid methyl ester

Inchi: InChI=1S/C21H32O2/c1-14-12-21-11-8-16-19(2,17(21)7-6-15(14)13-21)9-5-10-20(16,3)1

InchiKey: DWTRNJFPDXIFSY-UHFFFAOYSA-N

Formula: C21H32O2

SMILES: C=C1CC23CCC4C(C)(C(=O)OC)CCCC4(C)C2CCC1C3

Mol. weight [g/mol]: 316.48

CAS: 5524-25-4

Physical Properties

Property code	Value	Unit	Source
gf	107.81	kJ/mol	Joback Method
hf	-365.73	kJ/mol	Joback Method
hfus	19.16	kJ/mol	Joback Method
hvap	67.92	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	5.128		Crippen Method
mcvol	266.450	ml/mol	McGowan Method
pc	1625.91	kPa	Joback Method
rinpol	2286.00		NIST Webbook
rinpol	2313.70		NIST Webbook
rinpol	2285.00		NIST Webbook
rinpol	2270.00		NIST Webbook
rinpol	2242.00		NIST Webbook
rinpol	2242.00		NIST Webbook
rinpol	2270.00		NIST Webbook
rinpol	2292.00		NIST Webbook
rinpol	2291.00		NIST Webbook
rinpol	2313.70		NIST Webbook
tb	790.75	K	Joback Method
tc	1029.43	K	Joback Method
tf	533.17	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	890.86	J/mol×K	790.75	Joback Method
cpg	917.63	J/mol×K	830.53	Joback Method
cpg	944.60	J/mol×K	870.31	Joback Method
cpg	972.25	J/mol×K	910.09	Joback Method
cpg	1001.05	J/mol×K	949.87	Joback Method
cpg	1031.48	J/mol×K	989.65	Joback Method
cpg	1064.01	J/mol×K	1029.43	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5524254&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