Kaur-16-en-19-al

Inchi: InChI=1S/C20H30O/c1-14-11-20-10-7-16-18(2,13-21)8-4-9-19(16,3)17(20)6-5-15(14)12-

InchiKey: JCAVDWHQNFTFBW-UHFFFAOYSA-N

Formula: C20H30O

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

Mol. weight [g/mol]: 286.45

Physical Properties

Property code	Value	Unit	Source
gf	233.79	kJ/mol	Joback Method
hf	-185.87	kJ/mol	Joback Method
hfus	16.07	kJ/mol	Joback Method
hvap	63.26	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	5.154		Crippen Method
mcvol	246.490	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
rinpol	2330.00		NIST Webbook
rinpol	2361.00		NIST Webbook
tb	740.24	K	Joback Method
tc	982.40	K	Joback Method
tf	491.74	K	Joback Method
vc	0.945	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.94	J/mol×K	740.24	Joback Method
cpg	822.65	J/mol×K	780.60	Joback Method
cpg	848.11	J/mol×K	820.96	Joback Method
cpg	873.84	J/mol×K	861.32	Joback Method
cpg	900.34	J/mol×K	901.68	Joback Method
cpg	928.15	J/mol×K	942.04	Joback Method
cpg	957.77	J/mol×K	982.40	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=R195441&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