kauren-19-ol

Inchi: InChI=1S/C20H34O/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: YNHXWZNOUUQLCY-UHFFFAOYSA-N
Formula: C20H34O
SMILES: CC1CC23CCC4C(C)(CO)CCCC4(C)C2CCC1C3
Mol. weight [g/mol]: 290.48

Physical Properties

Property code	Value	Unit	Source
gf	135.70	kJ/mol	Joback Method
hf	-357.10	kJ/mol	Joback Method
hfus	20.10	kJ/mol	Joback Method
hvap	72.75	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	5.028		Crippen Method
mcvol	255.090	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	2290.00		NIST Webbook
rinpol	2290.00		NIST Webbook
tb	779.93	K	Joback Method
tc	1001.88	K	Joback Method
tf	492.64	K	Joback Method
vc	0.962	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.98	J/mol×K	779.93	Joback Method
cpg	903.39	J/mol×K	816.92	Joback Method
cpg	928.87	J/mol×K	853.91	Joback Method
cpg	954.80	J/mol×K	890.90	Joback Method
cpg	981.60	J/mol×K	927.89	Joback Method
cpg	1009.67	J/mol×K	964.89	Joback Method
cpg	1039.41	J/mol×K	1001.88	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=U143814&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume