ent-Kaurenal

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-FOEMKWDFSA-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	2249.00		NIST Webbook
rinpol	2257.00		NIST Webbook
rinpol	2257.00		NIST Webbook
rinpol	2258.00		NIST Webbook
rinpol	2231.00		NIST Webbook
rinpol	2233.00		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=R79127&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