serratane-l

Inchi: InChI=1S/C30H52/c1-26(2)15-8-17-29(6)22-11-13-25-28(5,20-21(22)10-12-23(26)29)19-
InchiKey: SKHPWXHRIDLXBT-RSNZLUEJSA-N
Formula: C30H52
SMILES: CC1(C)CCCC2(C)C3CCC4C(C)(CCC5C(C)(C)CCCC54C)CC3CCC12
Mol. weight [g/mol]: 412.73

Physical Properties

Property code	Value	Unit	Source
gf	342.67	kJ/mol	Joback Method
hf	-373.31	kJ/mol	Joback Method
hfus	21.20	kJ/mol	Joback Method
hvap	76.02	kJ/mol	Joback Method
log10ws	-9.44		Crippen Method
logp	9.278		Crippen Method
mcvol	379.260	ml/mol	McGowan Method
pc	983.93	kPa	Joback Method
rinpol	3134.00		NIST Webbook
rinpol	3134.00		NIST Webbook
tb	931.51	K	Joback Method
tc	1183.18	K	Joback Method
tf	587.70	K	Joback Method
vc	1.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1467.83	J/mol×K	931.51	Joback Method
cpg	1517.05	J/mol×K	973.46	Joback Method
cpg	1569.71	J/mol×K	1015.40	Joback Method
cpg	1626.67	J/mol×K	1057.35	Joback Method
cpg	1688.79	J/mol×K	1099.29	Joback Method
cpg	1756.95	J/mol×K	1141.24	Joback Method
cpg	1832.00	J/mol×K	1183.18	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=R244489&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