1-«beta»-H-Laurenane

Inchi: InChI=1S/C20H34/c1-14-7-6-10-18(4)12-9-16-17(2,3)13-19(5)11-8-15(14)20(16,18)19/h1
InchiKey: WMGLDMQBOZFFAW-NHZOGJPWSA-N
Formula: C20H34
SMILES: CC1CCCC2(C)CCC3C(C)(C)CC4(C)CCC1C324
Mol. weight [g/mol]: 274.48

Physical Properties

Property code	Value	Unit	Source
gf	279.13	kJ/mol	Joback Method
hf	-183.47	kJ/mol	Joback Method
hfus	11.82	kJ/mol	Joback Method
hvap	54.75	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	6.055		Crippen Method
mcvol	249.220	ml/mol	McGowan Method
pc	1649.77	kPa	Joback Method
rinpol	1953.00		NIST Webbook
rinpol	1925.00		NIST Webbook
ripol	2191.00		NIST Webbook
ripol	2229.00		NIST Webbook
tb	683.72	K	Joback Method
tc	924.96	K	Joback Method
tf	459.24	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	787.27	J/mol×K	683.72	Joback Method
cpg	815.43	J/mol×K	723.93	Joback Method
cpg	842.93	J/mol×K	764.13	Joback Method
cpg	870.40	J/mol×K	804.34	Joback Method
cpg	898.50	J/mol×K	844.55	Joback Method
cpg	927.86	J/mol×K	884.75	Joback Method

cpg	959.11	J/mol×K	924.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R27271&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume