

epi-Laurene

Inchi: InChI=1S/C20H32/c1-14-7-6-10-18(4)12-9-16-17(2,3)13-19(5)11-8-15(14)20(16,18)19/h8-13,15-17,19-20
InchiKey: TYDFDHZTDWVUJF-IAAPBBNJSA-N
Formula: C20H32
SMILES: CC1CCCC2(C)CCC3C(C)(C)CC4(C)CC=C1C324
Mol. weight [g/mol]: 272.47

Physical Properties

Property code	Value	Unit	Source
gf	307.17	kJ/mol	Joback Method
hf	-116.82	kJ/mol	Joback Method
hfus	11.58	kJ/mol	Joback Method
hvap	56.01	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	5.975		Crippen Method
mcvol	244.920	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
rinpol	1891.00		NIST Webbook
tb	692.53	K	Joback Method
tc	936.67	K	Joback Method
tf	476.76	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.21	J/molxK	692.53	Joback Method
cpg	788.76	J/molxK	733.22	Joback Method
cpg	814.91	J/molxK	773.91	Joback Method
cpg	841.35	J/molxK	814.60	Joback Method
cpg	868.72	J/molxK	855.29	Joback Method
cpg	897.71	J/molxK	895.98	Joback Method
cpg	928.97	J/molxK	936.67	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=R403524&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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

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