ent-Trachylobane

Inchi: InChI=1S/C20H32/c1-17(2)7-5-8-18(3)15(17)6-9-20-11-14-13(10-16(18)20)19(14,4)12-20
InchiKey: JTJZAWZRQPNBLR-OXGLGORBSA-N
Formula: C20H32
SMILES: CC1(C)CCCC2(C)C1CCC13CC4C(CC12)C4(C)C3
Mol. weight [g/mol]: 272.47

Physical Properties

Property code	Value	Unit	Source
gf	364.08	kJ/mol	Joback Method
hf	-98.35	kJ/mol	Joback Method
hfus	14.15	kJ/mol	Joback Method
hvap	54.32	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	5.665		Crippen Method
mcvol	238.360	ml/mol	McGowan Method
pc	1762.45	kPa	Joback Method
rinpol	1989.00		NIST Webbook
tb	681.92	K	Joback Method
tc	923.85	K	Joback Method
tf	484.22	K	Joback Method
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.87	J/mol×K	681.92	Joback Method
cpg	793.78	J/mol×K	722.24	Joback Method
cpg	820.10	J/mol×K	762.56	Joback Method
cpg	846.54	J/mol×K	802.89	Joback Method
cpg	873.80	J/mol×K	843.21	Joback Method
cpg	902.61	J/mol×K	883.53	Joback Method
cpg	933.65	J/mol×K	923.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R420430&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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