ent-Trachyloban-3-one

Inchi: InChI=1S/C20H30O/c1-17(2)14-5-8-20-10-13-12(19(13,4)11-20)9-15(20)18(14,3)7-6-16(
InchiKey: DVXUPVLGDAAEFK-GWSLHTCTSA-N
Formula: C20H30O
SMILES: CC1(C)C(=O)CCC2(C)C3CC4C5CC3(CCC12)CC45C
Mol. weight [g/mol]: 286.45

Physical Properties

Property code	Value	Unit	Source
gf	241.49	kJ/mol	Joback Method
hf	-236.05	kJ/mol	Joback Method
hfus	13.66	kJ/mol	Joback Method
hvap	58.57	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.844		Crippen Method
mcvol	239.930	ml/mol	McGowan Method
pc	1815.41	kPa	Joback Method
rinpol	2226.00		NIST Webbook
tb	749.74	K	Joback Method
tc	1002.18	K	Joback Method
tf	552.44	K	Joback Method
vc	0.928	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	811.53	J/mol×K	749.74	Joback Method
cpg	839.27	J/mol×K	791.81	Joback Method
cpg	867.62	J/mol×K	833.89	Joback Method
cpg	897.33	J/mol×K	875.96	Joback Method
cpg	929.14	J/mol×K	918.03	Joback Method
cpg	963.82	J/mol×K	960.11	Joback Method
cpg	1002.12	J/mol×K	1002.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R420425&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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