Caryophyllane-c

Inchi: InChI=1S/C15H28/c1-11-6-5-7-12(2)13-10-15(3,4)14(13)9-8-11/h11-14H,5-10H2,1-4H3
InchiKey: SITKOPDZOGHVLY-UHFFFAOYSA-N
Formula: C15H28
SMILES: CC1CCCC(C)C2CC(C)(C)C2CC1
Mol. weight [g/mol]: 208.38

Physical Properties

Property code	Value	Unit	Source
gf	107.80	kJ/mol	Joback Method
hf	-283.91	kJ/mol	Joback Method
hfus	17.29	kJ/mol	Joback Method
hvap	47.59	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.885		Crippen Method
mcvol	200.490	ml/mol	McGowan Method
pc	1846.75	kPa	Joback Method
rinpol	1450.00		NIST Webbook
ripol	1555.00		NIST Webbook
ripol	1555.00		NIST Webbook
tb	563.66	K	Joback Method
tc	784.20	K	Joback Method
tf	288.27	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.83	J/mol×K	563.66	Joback Method
cpg	569.05	J/mol×K	600.42	Joback Method
cpg	594.68	J/mol×K	637.17	Joback Method
cpg	618.83	J/mol×K	673.93	Joback Method
cpg	641.64	J/mol×K	710.68	Joback Method
cpg	663.22	J/mol×K	747.44	Joback Method
cpg	683.72	J/mol×K	784.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R306537&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