4-Desmethyl caryophylla-8(14)-en-5-one

Other names: des-4-Methyl-caryophyll-8(14)-en-5-one
4-Desmethylcaryophyll-8(14)-en-5-one
Inchi: InChI=1S/C14H22O/c1-10-7-8-11(15)5-4-6-13-12(10)9-14(13,2)3/h12-13H,1,4-9H2,2-3H
InchiKey: SVROROODYLVLSH-UHFFFAOYSA-N
Formula: C14H22O
SMILES: C=C1CCC(=O)CCCC2C1CC2(C)C
Mol. weight [g/mol]: 206.32

Physical Properties

Property code	Value	Unit	Source
gf	45.29	kJ/mol	Joback Method
hf	-276.05	kJ/mol	Joback Method
hfus	10.91	kJ/mol	Joback Method
hvap	50.39	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.738		Crippen Method
mcvol	183.670	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	1539.00		NIST Webbook
ripol	2020.00		NIST Webbook
ripol	2020.00		NIST Webbook
ripol	2020.00		NIST Webbook
tb	617.10	K	Joback Method
tc	857.50	K	Joback Method
tf	367.38	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.01	J/mol×K	617.10	Joback Method
cpg	533.52	J/mol×K	657.17	Joback Method
cpg	555.64	J/mol×K	697.23	Joback Method
cpg	576.51	J/mol×K	737.30	Joback Method

cpg	596.24	J/mol×K	777.37	Joback Method
cpg	614.97	J/mol×K	817.43	Joback Method
cpg	632.83	J/mol×K	857.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R336206&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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