Patchoulenone

Inchi: InChI=1S/C15H22O/c1-9-7-8-15-10(2)5-6-11(14(15,3)4)13(16)12(9)15/h10-11H,5-8H2,1-
InchiKey: JAWSHISYWRRQQQ-ZIBATOQPSA-N
Formula: C15H22O
SMILES: CC1=C2C(=O)C3CCC(C)C2(CC1)C3(C)C
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	102.89	kJ/mol	Joback Method
hf	-239.57	kJ/mol	Joback Method
hfus	13.24	kJ/mol	Joback Method
hvap	52.32	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.738		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2224.99	kPa	Joback Method
rinpol	1594.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1600.00		NIST Webbook
ripol	2089.00		NIST Webbook
tb	644.11	K	Joback Method
tc	883.54	K	Joback Method
tf	443.17	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.11	J/mol×K	644.11	Joback Method
cpg	562.10	J/mol×K	684.01	Joback Method
cpg	582.11	J/mol×K	723.92	Joback Method
cpg	601.45	J/mol×K	763.82	Joback Method
cpg	620.44	J/mol×K	803.73	Joback Method
cpg	639.37	J/mol×K	843.63	Joback Method

cpg	658.57	J/mol×K	883.54	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R334304&Units=SI

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