Patchoulyl acetate

Inchi: InChI=1S/C17H28O2/c1-11-6-9-17(19-12(2)18)15(3,4)13-7-8-16(17,5)14(11)10-13/h11,1
InchiKey: ZCUUERVRGQEHFO-CADBEIPOSA-N
Formula: C17H28O2
SMILES: CC(=O)OC12CCC(C)C3CC(CCC31C)C2(C)C
Mol. weight [g/mol]: 264.40

Physical Properties

Property code	Value	Unit	Source
gf	-23.21	kJ/mol	Joback Method
hf	-448.23	kJ/mol	Joback Method
hfus	17.10	kJ/mol	Joback Method
hvap	58.30	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.181		Crippen Method
mcvol	225.250	ml/mol	McGowan Method
pc	1845.16	kPa	Joback Method
rinpol	2001.00		NIST Webbook
rinpol	2001.00		NIST Webbook
rinpol	2001.00		NIST Webbook
tb	680.12	K	Joback Method
tc	906.53	K	Joback Method
tf	459.27	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	690.49	J/mol×K	680.12	Joback Method
cpg	713.37	J/mol×K	717.86	Joback Method
cpg	735.56	J/mol×K	755.59	Joback Method
cpg	757.45	J/mol×K	793.33	Joback Method
cpg	779.41	J/mol×K	831.06	Joback Method
cpg	801.82	J/mol×K	868.80	Joback Method
cpg	825.06	J/mol×K	906.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R224747&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