

Epifriedelinol (5B-methyl-friedelanol) acetate

Inchi: InChI=1S/C32H54O2/c1-21-23(34-22(2)33)10-11-24-29(21,6)13-12-25-30(24,7)17-19-32
InchiKey: NXKDUDYUASKXAY-VKQYTXUIISA-N
Formula: C32H54O2
SMILES: CC(=O)OC1CCC2C(C)(CCC3C2(C)CCC2(C)C4CC(C)(C)CCC4(C)CCC32C)C1C
Mol. weight [g/mol]: 470.77

Physical Properties

Property code	Value	Unit	Source
gf	124.49	kJ/mol	Joback Method
hf	-658.33	kJ/mol	Joback Method
hfus	26.04	kJ/mol	Joback Method
hvap	87.99	kJ/mol	Joback Method
log10ws	-9.25		Crippen Method
logp	8.820		Crippen Method
mcvol	414.880	ml/mol	McGowan Method
pc	892.67	kPa	Joback Method
rinsol	3457.00		NIST Webbook
tb	1044.86	K	Joback Method
tc	1296.57	K	Joback Method
tf	705.58	K	Joback Method
vc	1.562	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1739.31	J/molxK	1044.86	Joback Method
cpg	1807.68	J/molxK	1086.81	Joback Method
cpg	1883.02	J/molxK	1128.76	Joback Method
cpg	1966.34	J/molxK	1170.71	Joback Method
cpg	2058.60	J/molxK	1212.67	Joback Method
cpg	2160.78	J/molxK	1254.62	Joback Method
cpg	2273.87	J/molxK	1296.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R111176&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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