13-nor-Eudesm-5-en-11-one

Inchi: InChI=1S/C14H22O/c1-10-5-4-7-14(3)8-6-12(11(2)15)9-13(10)14/h9-10,12H,4-8H2,1-3H
InchiKey: SEPLFXIHUVTSIX-RCYCPFCNSA-N
Formula: C14H22O
SMILES: CC(=O)C1C=C2C(C)CCCC2(C)CC1
Mol. weight [g/mol]: 206.32

Physical Properties

Property code	Value	Unit	Source
gf	18.31	kJ/mol	Joback Method
hf	-282.70	kJ/mol	Joback Method
hfus	17.09	kJ/mol	Joback Method
hvap	53.51	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.738		Crippen Method
mcvol	183.670	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
rinpol	1540.00		NIST Webbook
rinpol	1547.00		NIST Webbook
rinpol	1540.00		NIST Webbook
tb	603.86	K	Joback Method
tc	831.60	K	Joback Method
tf	352.21	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.13	J/mol×K	603.86	Joback Method
cpg	518.51	J/mol×K	641.82	Joback Method
cpg	538.57	J/mol×K	679.77	Joback Method
cpg	557.47	J/mol×K	717.73	Joback Method
cpg	575.36	J/mol×K	755.68	Joback Method
cpg	592.39	J/mol×K	793.64	Joback Method
cpg	608.73	J/mol×K	831.60	Joback Method

Sources

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=R198326&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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