13-nor-cis-Eudesm-6-en-8-one

Inchi: InChI=1S/C14H22O/c1-4-11-8-12-10(2)6-5-7-14(12,3)9-13(11)15/h8,10,12H,4-7,9H2,1-3
InchiKey: SEOAUNZLBHTCGB-RCYCPFCNSA-N
Formula: C14H22O
SMILES: CCC1=CC2C(C)CCCC2(C)CC1=O
Mol. weight [g/mol]: 206.32

Physical Properties

Property code	Value	Unit	Source
gf	24.64	kJ/mol	Joback Method
hf	-307.82	kJ/mol	Joback Method
hfus	15.00	kJ/mol	Joback Method
hvap	51.01	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.738		Crippen Method
mcvol	183.670	ml/mol	McGowan Method
pc	2195.89	kPa	Joback Method
rinpol	1528.00		NIST Webbook
rinpol	1528.00		NIST Webbook
tb	617.81	K	Joback Method
tc	851.30	K	Joback Method
tf	370.50	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.02	J/mol×K	617.81	Joback Method
cpg	531.19	J/mol×K	656.73	Joback Method
cpg	552.11	J/mol×K	695.64	Joback Method
cpg	571.89	J/mol×K	734.56	Joback Method
cpg	590.67	J/mol×K	773.47	Joback Method
cpg	608.59	J/mol×K	812.39	Joback Method
cpg	625.77	J/mol×K	851.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R198653&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