11,12,13-tri-nor-cis-Eudesm-5-en-7-one

Other names: 11,12,13-tris-nor-cis-Eudesm-5-en-7-one
Inchi: InChI=1S/C12H18O/c1-9-4-3-6-12(2)7-5-10(13)8-11(9)12/h8-9H,3-7H2,1-2H3/t9-,12+/m0
InchiKey: KLTKQWRPJDRMTL-JOYOIKCWSA-N
Formula: C12H18O
SMILES: CC1CCCC2(C)CCC(=O)C=C12
Mol. weight [g/mol]: 178.27

Physical Properties

Property code	Value	Unit	Source
gf	15.51	kJ/mol	Joback Method
hf	-246.20	kJ/mol	Joback Method
hfus	8.75	kJ/mol	Joback Method
hvap	46.87	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.102		Crippen Method
mcvol	155.490	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
rinpol	1517.00		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1517.00		NIST Webbook
tb	576.72	K	Joback Method
tc	820.09	K	Joback Method
tf	352.20	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.28	J/mol×K	576.72	Joback Method
cpg	425.04	J/mol×K	617.28	Joback Method
cpg	444.48	J/mol×K	657.84	Joback Method
cpg	462.77	J/mol×K	698.41	Joback Method
cpg	480.04	J/mol×K	738.97	Joback Method
cpg	496.46	J/mol×K	779.53	Joback Method

cpg	512.16	J/mol×K	820.09	Joback Method

Sources

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=R198524&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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