11,12,13-tri-nor-cis-Eudesma-5,8-dien-7-one

Other names: 11,12,13-tris-nor-cis-Eudesma-5,8-dien-7-one
Inchi: InChI=1S/C12H16O/c1-9-4-3-6-12(2)7-5-10(13)8-11(9)12/h5,7-9H,3-4,6H2,1-2H3/t9-,12+
InchiKey: SPNLYFPIWOEXSG-JOYOIKCWSA-N
Formula: C12H16O
SMILES: CC1CCCC2(C)C=CC(=O)C=C12
Mol. weight [g/mol]: 176.25

Physical Properties

Property code	Value	Unit	Source
gf	45.47	kJ/mol	Joback Method
hf	-188.42	kJ/mol	Joback Method
hfus	9.97	kJ/mol	Joback Method
hvap	47.16	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.878		Crippen Method
mcvol	151.190	ml/mol	McGowan Method
pc	2850.52	kPa	Joback Method
rinpol	1540.00		NIST Webbook
rinpol	1536.00		NIST Webbook
ripol	2342.00		NIST Webbook
tb	575.88	K	Joback Method
tc	821.75	K	Joback Method
tf	352.96	K	Joback Method
vc	0.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.39	J/mol×K	575.88	Joback Method
cpg	403.89	J/mol×K	616.86	Joback Method
cpg	422.12	J/mol×K	657.84	Joback Method
cpg	439.24	J/mol×K	698.81	Joback Method
cpg	455.40	J/mol×K	739.79	Joback Method
cpg	470.76	J/mol×K	780.77	Joback Method

cpg	485.47	J/mol×K	821.75	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=R198539&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume