

24-Norursa-3,12-dien-11-one

Inchi:	InChI=1S/C29H44O/c1-18-10-13-26(4)15-16-28(6)22(24(26)20(18)3)17-23(30)25-27(5)1
InchiKey:	MRHRKEUKVNZEGQ-UHFFFAOYSA-N
Formula:	C29H44O
SMILES:	CC1=CCCC2(C)C1CCC1(C)C2C(=O)C=C2C3C(C)C(C)CCC3(C)CCC21C
Mol. weight [g/mol]:	408.66
CAS:	930591-92-7

Physical Properties

Property code	Value	Unit	Source
gf	277.62	kJ/mol	Joback Method
hf	-386.49	kJ/mol	Joback Method
hfus	27.11	kJ/mol	Joback Method
hvap	81.23	kJ/mol	Joback Method
log10ws	-8.25		Crippen Method
logp	7.763		Crippen Method
mcvol	358.140	ml/mol	McGowan Method
pc	1073.57	kPa	Joback Method
rinpol	3351.80		NIST Webbook
rinpol	3351.80		NIST Webbook
tb	984.89	K	Joback Method
tc	1241.17	K	Joback Method
tf	655.07	K	Joback Method
vc	1.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1396.93	J/molxK	984.89	Joback Method
cpg	1443.35	J/molxK	1027.60	Joback Method
cpg	1493.15	J/molxK	1070.32	Joback Method
cpg	1547.08	J/molxK	1113.03	Joback Method
cpg	1605.84	J/molxK	1155.74	Joback Method
cpg	1670.17	J/molxK	1198.45	Joback Method
cpg	1740.78	J/molxK	1241.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C930591927&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

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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