24-Norursa-3,9(11),12-triene

Inchi: InChI=1S/C29H44/c1-19-12-15-26(4)17-18-28(6)23(25(26)21(19)3)10-11-24-27(5)14-8-9
InchiKey: QSFCELCDWHMMTE-UHFFFAOYSA-N
Formula: C29H44
SMILES: CC1=CCCC2(C)C3=CC=C4C5C(C)C(C)CCC5(C)CCC4(C)C3(C)CCC12
Mol. weight [g/mol]: 392.66
CAS: 930591-91-6

Physical Properties

Property code	Value	Unit	Source
gf	428.25	kJ/mol	Joback Method
hf	-182.14	kJ/mol	Joback Method
hfus	27.36	kJ/mol	Joback Method
hvap	78.25	kJ/mol	Joback Method
log10ws	-9.06		Crippen Method
logp	8.504		Crippen Method
mcvol	352.270	ml/mol	McGowan Method
pc	1087.06	kPa	Joback Method
rinpol	3042.70		NIST Webbook
tb	925.88	K	Joback Method
tc	1175.47	K	Joback Method
tf	604.37	K	Joback Method
vc	1.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1297.55	J/mol×K	925.88	Joback Method
cpg	1338.79	J/mol×K	967.48	Joback Method
cpg	1382.74	J/mol×K	1009.08	Joback Method
cpg	1430.11	J/mol×K	1050.68	Joback Method
cpg	1481.63	J/mol×K	1092.27	Joback Method
cpg	1538.01	J/mol×K	1133.87	Joback Method
cpg	1599.97	J/mol×K	1175.47	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C930591916&Units=SI

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