24-Norursa-3,12-diene

Inchi: InChI=1S/C29H46/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: PSESUFHNSONVFL-UHFFFAOYSA-N
Formula: C29H46
SMILES: CC1=CCCC2(C)C1CCC1(C)C2CC=C2C3C(C)C(C)CCC3(C)CCC21C
Mol. weight [g/mol]: 394.68
CAS: 201358-25-0

Physical Properties

Property code	Value	Unit	Source
gf	400.21	kJ/mol	Joback Method
hf	-248.79	kJ/mol	Joback Method
hfus	27.60	kJ/mol	Joback Method
hvap	76.98	kJ/mol	Joback Method
log10ws	-8.97		Crippen Method
logp	8.584		Crippen Method
mcvol	356.570	ml/mol	McGowan Method
pc	1049.37	kPa	Joback Method
rinpol	3105.60		NIST Webbook
tb	917.07	K	Joback Method
tc	1164.44	K	Joback Method
tf	586.85	K	Joback Method
vc	1.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1328.30	J/mol×K	917.07	Joback Method
cpg	1369.66	J/mol×K	958.30	Joback Method
cpg	1413.36	J/mol×K	999.53	Joback Method
cpg	1460.11	J/mol×K	1040.75	Joback Method
cpg	1510.59	J/mol×K	1081.98	Joback Method
cpg	1565.52	J/mol×K	1123.21	Joback Method
cpg	1625.58	J/mol×K	1164.44	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=C201358250&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