24-Noroleana-3,12-diene

Inchi: InChI=1S/C29H46/c1-20-9-8-13-27(5)21(20)12-14-29(7)24(27)11-10-22-23-19-25(2,3)15
InchiKey: BUSIZDBOZRBEOT-UHFFFAOYSA-N
Formula: C29H46
SMILES: CC1=CCCC2(C)C1CCC1(C)C2CC=C2C3CC(C)(C)CCC3(C)CCC21C
Mol. weight [g/mol]: 394.68
CAS: 201358-24-9

Physical Properties

Property code	Value	Unit	Source
gf	402.43	kJ/mol	Joback Method
hf	-213.21	kJ/mol	Joback Method
hfus	20.23	kJ/mol	Joback Method
hvap	76.14	kJ/mol	Joback Method
log10ws	-9.21		Crippen Method
logp	8.728		Crippen Method
mcvol	356.570	ml/mol	McGowan Method
pc	1104.47	kPa	Joback Method
rinpol	3057.50		NIST Webbook
tb	921.98	K	Joback Method
tc	1176.04	K	Joback Method
tf	614.99	K	Joback Method
vc	1.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1326.58	J/mol×K	921.98	Joback Method
cpg	1372.72	J/mol×K	964.32	Joback Method
cpg	1422.71	J/mol×K	1006.67	Joback Method
cpg	1477.47	J/mol×K	1049.01	Joback Method
cpg	1537.89	J/mol×K	1091.35	Joback Method
cpg	1604.88	J/mol×K	1133.69	Joback Method
cpg	1679.35	J/mol×K	1176.04	Joback Method

Sources

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=C201358249&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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