

17«beta»(H),21«alpha»(H)-30-Normoretane

Inchi:	InChI=1S/C29H50/c1-8-20-12-17-26(4)21(20)13-18-28(6)23(26)10-11-24-27(5)16-9-15-2
InchiKey:	XKJROQIFLGXWEY-NUYNIGSJSA-N
Formula:	C29H50
SMILES:	CCC1CCC2(C)C1CCC1(C)C2CCC2C3(C)CCCC(C)(C)C3CCC21C
Mol. weight [g/mol]:	398.71

Physical Properties

Property code	Value	Unit	Source
gf	358.45	kJ/mol	Joback Method
hf	-340.35	kJ/mol	Joback Method
hfus	22.81	kJ/mol	Joback Method
hvap	73.44	kJ/mol	Joback Method
log10ws	-9.02		Crippen Method
logp	8.888		Crippen Method
mvol	365.170	ml/mol	McGowan Method
pc	1012.95	kPa	Joback Method
rinpol	3017.00		NIST Webbook
rinpol	3017.00		NIST Webbook
tb	900.09	K	Joback Method
tc	1143.83	K	Joback Method
tf	583.47	K	Joback Method
vc	1.381	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1379.44	J/molxK	900.09	Joback Method
cpg	1424.12	J/molxK	940.71	Joback Method
cpg	1471.71	J/molxK	981.34	Joback Method
cpg	1523.01	J/molxK	1021.96	Joback Method
cpg	1578.84	J/molxK	1062.58	Joback Method
cpg	1639.98	J/molxK	1103.20	Joback Method
cpg	1707.26	J/molxK	1143.83	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=R548573&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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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