

18-«beta»-H-30-nor-Moretane

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-FNHDSZEQSA-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
hfus	22.81	kJ/mol	Joback Method
logp	8.888		Crippen Method
mcpvol	365.170	ml/mol	McGowan Method
rinpol	3048.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1379.44	J/mol×K	900.09	Joback Method
cpg	1424.12	J/mol×K	940.71	Joback Method
cpg	1471.71	J/mol×K	981.34	Joback Method
cpg	1523.01	J/mol×K	1021.96	Joback Method
cpg	1578.84	J/mol×K	1062.58	Joback Method
cpg	1639.98	J/mol×K	1103.20	Joback Method
cpg	1707.26	J/mol×K	1143.83	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R214507&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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