D:a-friedooleanane

Other names:	Friedelane
Inchi:	Friedelane, docosahydro-2,2,4a,6a,8a,9,12b,14a-octamethyl-, [4aR-(4a«alpha»,6a«alpha»,6b«beta»,8a«alpha»,9«alpha»,12a«beta»,12b«alpha»,14a« Picene, docosahydro-2,2,4a,6a,8a,9,12b,14a-octamethyl-, [4aR-(4a«alpha»,6a«alpha»,6b«beta»,8a«alpha»,9«alpha»,12a«beta»,12b«alpha»,14a« InChI=1S/C30H52/c1-21-10-9-11-22-27(21,5)13-12-23-28(22,6)17-19-30(8)24-20-25(2,3
InchiKey:	KVSNMTUIMXZPLU-UTHRLOSQSA-N
Formula:	C30H52
SMILES:	C[C@@H]1CCCC2[C@@]3(C)CC[C@]4(C)C5CC(C)(C)CC[C@@]5(C)CC[C@@]4(C)C
Mol. weight [g/mol]:	412.75

Physical Properties

Property code	Value	Unit	Source
hfus	17.00	kJ/mol	Joback Method
logp	9.278		Crippen Method
mcvol	379.260	ml/mol	McGowan Method
rinpol	3155.00		NIST Webbook
rinpol	3155.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1461.58	J/mol×K	927.48	Joback Method
cpg	1514.42	J/mol×K	969.58	Joback Method
cpg	1571.97	J/mol×K	1011.69	Joback Method
cpg	1635.26	J/mol×K	1053.79	Joback Method
cpg	1705.30	J/mol×K	1095.89	Joback Method
cpg	1783.11	J/mol×K	1137.99	Joback Method
cpg	1869.72	J/mol×K	1180.10	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C559739&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
rinpol:	Non-polar retention indices

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