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:	CC1CCCC2C1(C)CCC1C2(C)CCC2(C)C3CC(C)(C)CCC3(C)CCC12C
Mol. weight [g/mol]:	412.73
CAS:	559-73-9

Physical Properties

Property code	Value	Unit	Source
gf	349.28	kJ/mol	Joback Method
hf	-351.91	kJ/mol	Joback Method
hfus	17.00	kJ/mol	Joback Method
hvap	74.69	kJ/mol	Joback Method
log10ws	-9.44		Crippen Method
logp	9.278		Crippen Method
mcvol	379.260	ml/mol	McGowan Method
pc	996.39	kPa	Joback Method
rinpol	3155.00		NIST Webbook
rinpol	3155.00		NIST Webbook
tb	927.48	K	Joback Method
tc	1180.10	K	Joback Method
tf	615.12	K	Joback Method
vc	1.427	m3/kmol	Joback Method

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C559739&Units=SI

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