taraxastane

Inchi: InChI=1S/C30H50/c1-20-12-16-27(5)18-19-29(7)22(25(27)21(20)2)10-11-24-28(6)15-9-1
InchiKey: XJQCFWLHTAYWAT-DAHABVLQSA-N
Formula: C30H50
SMILES: C=C1CCC2(C)CCC3(C)C(CCC4C5(C)CCCC(C)(C)C5CCC43C)C2C1C
Mol. weight [g/mol]: 410.72

Physical Properties

Property code	Value	Unit	Source
gf	407.85	kJ/mol	Joback Method
hf	-282.91	kJ/mol	Joback Method
hfus	22.14	kJ/mol	Joback Method
hvap	76.00	kJ/mol	Joback Method
log10ws	-9.29		Crippen Method
logp	9.054		Crippen Method
mcvol	374.960	ml/mol	McGowan Method
pc	980.23	kPa	Joback Method
rinpol	3177.00		NIST Webbook
rinpol	3177.00		NIST Webbook
tb	926.40	K	Joback Method
tc	1173.87	K	Joback Method
tf	604.90	K	Joback Method
vc	1.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1429.59	J/mol×K	926.40	Joback Method
cpg	1476.85	J/mol×K	967.65	Joback Method
cpg	1527.47	J/mol×K	1008.89	Joback Method
cpg	1582.29	J/mol×K	1050.14	Joback Method
cpg	1642.12	J/mol×K	1091.38	Joback Method
cpg	1707.79	J/mol×K	1132.63	Joback Method
cpg	1780.13	J/mol×K	1173.87	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=R244503&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