C27 18A-Hopane II (Ts)

Inchi: InChI=1S/C27H46/c1-23(2)14-8-16-25(4)20(23)13-18-27(6)22(25)11-10-21-24(3)15-7-9-1
InchiKey: WPKYQECPNNWDJY-QJUJFBOWSA-N
Formula: C27H46
SMILES: CC1(C)CCCC2(C)C1CCC1(C)C2CCC2C3(C)CCCC3CCC21C
Mol. weight [g/mol]: 370.65

Physical Properties

Property code	Value	Unit	Source
gf	349.32	kJ/mol	Joback Method
hf	-278.73	kJ/mol	Joback Method
hfus	16.56	kJ/mol	Joback Method
hvap	69.30	kJ/mol	Joback Method
log10ws	-8.42		Crippen Method
logp	8.252		Crippen Method
mcvol	336.990	ml/mol	McGowan Method
pc	1175.24	kPa	Joback Method
rinpol	2856.00		NIST Webbook
tb	859.00	K	Joback Method
tc	1110.54	K	Joback Method
tf	565.17	K	Joback Method
vc	1.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1233.99	J/mol×K	859.00	Joback Method
cpg	1275.45	J/mol×K	900.92	Joback Method
cpg	1319.40	J/mol×K	942.85	Joback Method
cpg	1366.73	J/mol×K	984.77	Joback Method
cpg	1418.31	J/mol×K	1026.69	Joback Method
cpg	1475.05	J/mol×K	1068.61	Joback Method
cpg	1537.82	J/mol×K	1110.54	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=R56101&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