(1S,4aS,4bS,7S,8aS,10aS)-7-Isopropyl-1,4a-dimetl

Inchi: InChI=1S/C19H34/c1-13(2)15-7-10-18-16(12-15)8-9-17-14(3)6-5-11-19(17,18)4/h13-18H
InchiKey: HTNCYKZTYXSRHL-MGYGNFHQSA-N
Formula: C19H34
SMILES: CC(C)C1CCC2C(CCC3C(C)CCCC32C)C1
Mol. weight [g/mol]: 262.47
CAS: 2221-95-6

Physical Properties

Property code	Value	Unit	Source
gf	199.79	kJ/mol	Joback Method
hf	-298.95	kJ/mol	Joback Method
hfus	22.26	kJ/mol	Joback Method
hvap	56.02	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	5.911		Crippen Method
mcvol	245.990	ml/mol	McGowan Method
pc	1510.50	kPa	Joback Method
rinpol	1941.70		NIST Webbook
rinpol	1941.70		NIST Webbook
tb	661.48	K	Joback Method
tc	885.70	K	Joback Method
tf	336.29	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	759.74	J/mol×K	661.48	Joback Method
cpg	788.60	J/mol×K	698.85	Joback Method
cpg	815.79	J/mol×K	736.22	Joback Method
cpg	841.48	J/mol×K	773.59	Joback Method
cpg	865.85	J/mol×K	810.96	Joback Method
cpg	889.09	J/mol×K	848.33	Joback Method
cpg	911.38	J/mol×K	885.70	Joback Method

Sources

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=C2221956&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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