

(4aR,6aS,10aS,10bR)-3,4a,7,7,10a-Pentamethyl-4a

Inchi:	InChI=1S/C18H30O/c1-13-7-8-15-17(4)11-6-10-16(2,3)14(17)9-12-18(15,5)19-13/h7,14-
InchiKey:	LAEIZWJAQRGPDA-UHFFFAOYSA-N
Formula:	C18H30O
SMILES:	CC1=CCC2C(C)(CCC3C(C)(C)CCCC32C)O1
Mol. weight [g/mol]:	262.43
CAS:	5153-92-4

Physical Properties

Property code	Value	Unit	Source
gf	124.75	kJ/mol	Joback Method
hf	-307.90	kJ/mol	Joback Method
hfus	18.34	kJ/mol	Joback Method
hvap	57.65	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	5.312		Crippen Method
mvol	233.470	ml/mol	McGowan Method
pc	1810.77	kPa	Joback Method
rinpol	1894.20		NIST Webbook
tb	675.28	K	Joback Method
tc	916.40	K	Joback Method
tf	431.91	K	Joback Method
vc	0.874	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.28	J/molxK	675.28	Joback Method
cpg	734.11	J/molxK	715.47	Joback Method
cpg	759.02	J/molxK	755.65	Joback Method
cpg	783.44	J/molxK	795.84	Joback Method
cpg	807.83	J/molxK	836.02	Joback Method
cpg	832.65	J/molxK	876.21	Joback Method
cpg	858.34	J/molxK	916.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5153924&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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