1H-3a,7-Methanoazulene, octahydro-1,4,9,9-tetramethyl-

Other names: Patchulane
Inchi: InChI=1S/C15H26/c1-10-7-8-15-11(2)5-6-12(9-13(10)15)14(15,3)4/h10-13H,5-9H2,1-4H3
InchiKey: MVZZUMCHPFHUOS-UHFFFAOYSA-N
Formula: C15H26
SMILES: CC1CCC23C(C)CCC(CC12)C3(C)C
Mol. weight [g/mol]: 206.37
CAS: 19078-35-4

Physical Properties

Property code	Value	Unit	Source
gf	199.36	kJ/mol	Joback Method
hf	-177.39	kJ/mol	Joback Method
hfus	15.43	kJ/mol	Joback Method
hvap	45.84	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	4.495		Crippen Method
mcvol	189.630	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
ripol	1890.00		NIST Webbook
tb	557.83	K	Joback Method
tc	780.06	K	Joback Method
tf	340.67	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.52	J/mol×K	557.83	Joback Method
cpg	547.59	J/mol×K	594.87	Joback Method
cpg	570.94	J/mol×K	631.91	Joback Method
cpg	592.86	J/mol×K	668.95	Joback Method
cpg	613.64	J/mol×K	705.99	Joback Method
cpg	633.54	J/mol×K	743.02	Joback Method
cpg	652.86	J/mol×K	780.06	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=C19078354&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume