Aciphyllene

Other names:	(5R,8S,8aS)-3,8-Dimethyl-5-(prop-1-en-2-yl)-1,2,4,5,6,7,8,8a-octahydroazulene Guaia-4,11-diene
Inchi:	InChI=1S/C15H24/c1-10(2)13-7-5-11(3)14-8-6-12(4)15(14)9-13/h11,13-14H,1,5-9H2,2-4
InchiKey:	YIWKBKBHKZAWQV-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	C=C(C)C1CCC(C)C2CCC(C)=C2C1
Mol. weight [g/mol]:	204.35
CAS:	87745-31-1

Physical Properties

Property code	Value	Unit	Source
gf	230.80	kJ/mol	Joback Method
hf	-101.83	kJ/mol	Joback Method
hfus	21.40	kJ/mol	Joback Method
hvap	50.22	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1927.05	kPa	Joback Method
rinpol	1499.00		NIST Webbook
tb	574.17	K	Joback Method
tc	791.30	K	Joback Method
tf	286.45	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.80	J/mol×K	574.17	Joback Method
cpg	525.03	J/mol×K	610.36	Joback Method
cpg	546.90	J/mol×K	646.55	Joback Method
cpg	567.47	J/mol×K	682.74	Joback Method
cpg	586.78	J/mol×K	718.92	Joback Method
cpg	604.90	J/mol×K	755.11	Joback Method

cpg	621.88	J/mol×K	791.30	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=C87745311&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