

Pacifigorgia-2(10),11-diene

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H24/c1-10(2)9-15-12(4)5-7-13-11(3)6-8-14(13)15/h9,11-14H,1,5-8H2,2-4H

LOWXYGTWKXWTGY-WRCLNMPESA-N

C15H24

C=C(C)C=C1C(C)CCC2C(C)CCC12

204.35

Physical Properties

Property code	Value	Unit	Source
gf	269.95	kJ/mol	Joback Method
hf	-74.82	kJ/mol	Joback Method
hfus	24.45	kJ/mol	Joback Method
hvap	48.91	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.581		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1869.17	kPa	Joback Method
rinpol	1435.00		NIST Webbook
rinpol	1435.00		NIST Webbook
tb	562.75	K	Joback Method
tc	775.05	K	Joback Method
tf	270.29	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.24	J/mol×K	562.75	Joback Method
cpg	523.61	J/mol×K	598.13	Joback Method
cpg	545.61	J/mol×K	633.52	Joback Method
cpg	566.31	J/mol×K	668.90	Joback Method
cpg	585.77	J/mol×K	704.28	Joback Method
cpg	604.06	J/mol×K	739.66	Joback Method
cpg	621.23	J/mol×K	775.05	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=R332100&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
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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