

epi-Bicyclophellandrene

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H24/c1-11-7-5-6-8-12(2)14-13(10-9-11)15(14,3)4/h7-8,13-14H,5-6,9-10H2

GWWKHRPQDGQFPK-NTLHZVPKSA-N

C15H24

CC1=CCCC=C(C)C2C(CC1)C2(C)C

204.35

Physical Properties

Property code	Value	Unit	Source
gf	163.88	kJ/mol	Joback Method
hf	-150.61	kJ/mol	Joback Method
hfus	16.82	kJ/mol	Joback Method
hvap	50.12	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinpol	1436.00		NIST Webbook
rinpol	1423.00		NIST Webbook
rinpol	1423.00		NIST Webbook
tb	581.28	K	Joback Method
tc	808.29	K	Joback Method
tf	323.31	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.31	J/mol×K	581.28	Joback Method
cpg	526.59	J/mol×K	619.11	Joback Method
cpg	548.47	J/mol×K	656.95	Joback Method
cpg	569.08	J/mol×K	694.78	Joback Method
cpg	588.58	J/mol×K	732.62	Joback Method
cpg	607.10	J/mol×K	770.45	Joback Method
cpg	624.78	J/mol×K	808.29	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=R409057&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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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