Copaane

Inchi: InChI=1S/C15H26/c1-9(2)11-7-8-15(4)12-6-5-10(3)14(15)13(11)12/h9-14H,5-8H2,1-4H3/
InchiKey: LJVYOZJXUGFDJA-DVZSBNJSSA-N
Formula: C15H26
SMILES: CC(C)C1CCC2(C)C3CCC(C)C2C13
Mol. weight [g/mol]: 206.37

Physical Properties

Property code	Value	Unit	Source
gf	214.51	kJ/mol	Joback Method
hf	-191.75	kJ/mol	Joback Method
hfus	20.30	kJ/mol	Joback Method
hvap	46.43	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	4.351		Crippen Method
mcvol	189.630	ml/mol	McGowan Method
pc	1908.57	kPa	Joback Method
rinpol	1455.00		NIST Webbook
rinpol	1421.00		NIST Webbook
rinpol	1477.00		NIST Webbook
rinpol	1437.00		NIST Webbook
ripol	1550.00		NIST Webbook
ripol	1599.00		NIST Webbook
tb	552.88	K	Joback Method
tc	763.56	K	Joback Method
tf	305.29	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.89	J/mol×K	552.88	Joback Method
cpg	546.37	J/mol×K	587.99	Joback Method
cpg	569.28	J/mol×K	623.11	Joback Method
cpg	590.81	J/mol×K	658.22	Joback Method

cpg	611.11	J/mol×K	693.33	Joback Method
cpg	630.35	J/mol×K	728.44	Joback Method
cpg	648.71	J/mol×K	763.56	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=R134159&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume