Cubebene

Inchi: InChI=1S/C15H24/c1-9(2)12-6-5-11(4)15-8-7-10(3)13(15)14(12)15/h7,9,11-14H,5-6,8H2
InchiKey: XUEHVOLRMXNRKQ-VGVBULKLSA-N
Formula: C15H24
SMILES: CC1=CCC23C(C)CCC(C(C)C)C2C13
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	242.55	kJ/mol	Joback Method
hf	-125.10	kJ/mol	Joback Method
hfus	20.07	kJ/mol	Joback Method
hvap	47.69	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.271		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	1352.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1334.00		NIST Webbook
ripol	1708.00		NIST Webbook
tb	561.69	K	Joback Method
tc	775.53	K	Joback Method
tf	322.81	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.35	J/mol×K	561.69	Joback Method
cpg	525.87	J/mol×K	597.33	Joback Method
cpg	546.93	J/mol×K	632.97	Joback Method
cpg	566.70	J/mol×K	668.61	Joback Method
cpg	585.36	J/mol×K	704.25	Joback Method
cpg	603.09	J/mol×K	739.89	Joback Method

cpg	620.07	J/mol×K	775.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R203097&Units=SI
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

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