1,2-Dihydrocuparene

Inchi: InChI=1S/C15H24/c1-12-6-8-13(9-7-12)15(4)11-5-10-14(15,2)3/h6-8,13H,5,9-11H2,1-4H
InchiKey: WVRVMHCZDFFAFB-UHFFFAOYSA-N
Formula: C15H24
SMILES: CC1=CCC(C2(C)CCCC2(C)C)C=C1
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	168.02	kJ/mol	Joback Method
hf	-123.90	kJ/mol	Joback Method
hfus	10.91	kJ/mol	Joback Method
hvap	48.30	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinpol	1521.00		NIST Webbook
tb	576.54	K	Joback Method
tc	811.87	K	Joback Method
tf	334.69	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.15	J/mol×K	576.54	Joback Method
cpg	524.71	J/mol×K	615.76	Joback Method
cpg	546.72	J/mol×K	654.98	Joback Method
cpg	567.48	J/mol×K	694.20	Joback Method
cpg	587.25	J/mol×K	733.43	Joback Method
cpg	606.33	J/mol×K	772.65	Joback Method
cpg	624.97	J/mol×K	811.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U414987&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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