1,4-Dihydrocuparene

Inchi: InChI=1S/C15H24/c1-12-6-8-13(9-7-12)15(4)11-5-10-14(15,2)3/h6-9,12-13H,5,10-11H2,1
InchiKey: JJSVVKVELWQYTN-UHFFFAOYSA-N
Formula: C15H24
SMILES: CC1C=CC(C2(C)CCCC2(C)C)C=C1
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	169.94	kJ/mol	Joback Method
hf	-132.77	kJ/mol	Joback Method
hfus	12.37	kJ/mol	Joback Method
hvap	47.33	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.581		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2110.00	kPa	Joback Method
rinpol	1530.90		NIST Webbook
rinpol	1530.90		NIST Webbook
tb	566.89	K	Joback Method
tc	801.17	K	Joback Method
tf	317.93	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.09	J/mol×K	566.89	Joback Method
cpg	525.59	J/mol×K	605.94	Joback Method
cpg	548.44	J/mol×K	644.98	Joback Method
cpg	569.91	J/mol×K	684.03	Joback Method
cpg	590.28	J/mol×K	723.08	Joback Method
cpg	609.83	J/mol×K	762.12	Joback Method
cpg	628.82	J/mol×K	801.17	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=U414986&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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