

Cedrene-V6

Inchi:	InChI=1S/C15H24/c1-6-15(5)10-7-12-11(2)14(3,4)9-8-13(12)15/h6,13H,1,7-10H2,2-5H3
InchiKey:	HNELXVYQXJWDON-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	<chem>C=CC1(C)CCC2=C(C)C(C)(C)CCC21</chem>
Mol. weight [g/mol]:	204.35

Physical Properties

Property code	Value	Unit	Source
gf	240.47	kJ/mol	Joback Method
hf	-55.40	kJ/mol	Joback Method
hfus	12.21	kJ/mol	Joback Method
hvap	47.66	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
tb	570.50	K	Joback Method
tc	793.44	K	Joback Method
tf	351.73	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.64	J/molxK	570.50	Joback Method
cpg	519.26	J/molxK	607.66	Joback Method
cpg	539.52	J/molxK	644.81	Joback Method
cpg	558.67	J/molxK	681.97	Joback Method
cpg	576.96	J/molxK	719.12	Joback Method
cpg	594.65	J/molxK	756.28	Joback Method
cpg	611.99	J/molxK	793.44	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=U162768&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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