«alpha»-cedrenal

Inchi: InChI=1S/C15H22O/c1-10-4-5-13-14(2,3)12-8-15(10,13)7-6-11(12)9-16/h6,9-10,12-13H,
InchiKey: OETRFUZAVAFOBR-SUTJQRNSSA-N
Formula: C15H22O
SMILES: CC1CCC2C(C)(C)C3CC12CC=C3C=O
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	127.88	kJ/mol	Joback Method
hf	-196.32	kJ/mol	Joback Method
hfus	17.48	kJ/mol	Joback Method
hvap	53.82	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.594		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2269.73	kPa	Joback Method
ripol	2217.00		NIST Webbook
tb	615.30	K	Joback Method
tc	842.99	K	Joback Method
tf	400.19	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.87	J/mol×K	615.30	Joback Method
cpg	551.35	J/mol×K	653.25	Joback Method
cpg	570.61	J/mol×K	691.20	Joback Method
cpg	588.97	J/mol×K	729.15	Joback Method
cpg	606.73	J/mol×K	767.10	Joback Method
cpg	624.18	J/mol×K	805.04	Joback Method
cpg	641.63	J/mol×K	842.99	Joback Method

Sources

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=R338871&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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