Alpha cis ocimene

Inchi: InChI=1S/C10H16/c1-5-10(4)8-6-7-9(2)3/h5,8H,1-2,6-7H2,3-4H3/b10-8-
InchiKey: XJPBRODHZKDRCB-NTMALXAHSA-N
Formula: C10H16
SMILES: C=CC(C)=CCCC(=C)C
Mol. weight [g/mol]: 136.23
CAS: 6874-44-8

Physical Properties

Property code	Value	Unit	Source
gf	272.12	kJ/mol	Joback Method
hf	98.77	kJ/mol	Joback Method
hfus	16.68	kJ/mol	Joback Method
hvap	36.63	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.475		Crippen Method
mcvol	138.860	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
tb	425.48	K	Joback Method
tc	609.58	K	Joback Method
tf	165.94	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.94	J/mol×K	425.48	Joback Method
cpg	282.35	J/mol×K	456.16	Joback Method
cpg	296.03	J/mol×K	486.85	Joback Method
cpg	309.00	J/mol×K	517.53	Joback Method
cpg	321.31	J/mol×K	548.21	Joback Method
cpg	332.99	J/mol×K	578.90	Joback Method
cpg	344.07	J/mol×K	609.58	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=C6874448&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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