

trans-Alloocimene

Other names:	(E)-Alloocimene
Inchi:	InChI=1S/C10H16/c1-5-10(4)8-6-7-9(2)3/h5-8H,1-4H3/b8-6+,10-5+
InchiKey:	GQVMHMFVWSSPF-SOYUKNQ TSA-N
Formula:	C10H16
SMILES:	CC=C(C)C=CC=C(C)C
Mol. weight [g/mol]:	136.23
CAS:	14947-20-7

Physical Properties

Property code	Value	Unit	Source
gf	256.88	kJ/mol	Joback Method
hf	82.35	kJ/mol	Joback Method
hfus	19.64	kJ/mol	Joback Method
hvap	37.89	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.475		Crippen Method
mcvol	138.860	ml/mol	McGowan Method
pc	2470.27	kPa	Joback Method
rinpol	1118.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1129.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1120.40		NIST Webbook
rinpol	1119.80		NIST Webbook
rinpol	1118.70		NIST Webbook
ripol	1402.80		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1396.00		NIST Webbook
ripol	1409.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1405.00		NIST Webbook
ripol	1409.00		NIST Webbook
ripol	1403.00		NIST Webbook

ripol	1396.00		NIST Webbook
ripol	1392.10		NIST Webbook
tb	440.44	K	Joback Method
tc	635.07	K	Joback Method
tf	159.30	K	Joback Method
vc	0.537	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.43	J/mol×K	440.44	Joback Method
cpg	284.46	J/mol×K	472.88	Joback Method
cpg	298.62	J/mol×K	505.32	Joback Method
cpg	311.96	J/mol×K	537.75	Joback Method
cpg	324.52	J/mol×K	570.19	Joback Method
cpg	336.36	J/mol×K	602.63	Joback Method
cpg	347.53	J/mol×K	635.07	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=C14947207&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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