Carane, 4,5-epoxy-, trans

Other names: 4,5-Epoxycarene
Inchi: InChI=1S/C10H16O/c1-5-4-6-7(10(6,2)3)9-8(5)11-9/h5-9H,4H2,1-3H3
InchiKey: KNHFDBGGSOSGEO-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CC1CC2C(C3OC13)C2(C)C
Mol. weight [g/mol]: 152.23
CAS: 6909-20-2

Physical Properties

Property code	Value	Unit	Source
gf	112.93	kJ/mol	Joback Method
hf	-202.95	kJ/mol	Joback Method
hfus	23.05	kJ/mol	Joback Method
hvap	39.85	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	2.066		Crippen Method
mcvol	125.050	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
rinpol	1179.00		NIST Webbook
rinpol	1179.00		NIST Webbook
tb	457.33	K	Joback Method
tc	662.18	K	Joback Method
tf	297.55	K	Joback Method
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.61	J/mol×K	457.33	Joback Method
cpg	326.70	J/mol×K	491.47	Joback Method
cpg	344.31	J/mol×K	525.61	Joback Method
cpg	360.60	J/mol×K	559.76	Joback Method
cpg	375.70	J/mol×K	593.90	Joback Method
cpg	389.78	J/mol×K	628.04	Joback Method

cpg	403.00	J/mol×K	662.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6909202&Units=SI
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

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