Carene, 3,4-epoxide

Inchi: InChI=1S/C10H16O/c1-9(2)6-4-8-10(3,11-8)5-7(6)9/h6-8H,4-5H2,1-3H3/t6-,7+,8?,10?/m
InchiKey: AGHSZSJVJPSERC-CCSIGSMKSA-N
Formula: C10H16O
SMILES: CC12CC3C(CC1O2)C3(C)C
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	115.15	kJ/mol	Joback Method
hf	-167.37	kJ/mol	Joback Method
hfus	15.69	kJ/mol	Joback Method
hvap	39.01	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.210		Crippen Method
mcvol	125.050	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
rinpol	1131.00		NIST Webbook
rinpol	1131.00		NIST Webbook
ripol	1438.00		NIST Webbook
tb	462.24	K	Joback Method
tc	676.49	K	Joback Method
tf	325.69	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.28	J/mol×K	462.24	Joback Method
cpg	327.25	J/mol×K	497.95	Joback Method
cpg	344.37	J/mol×K	533.66	Joback Method
cpg	359.91	J/mol×K	569.37	Joback Method
cpg	374.13	J/mol×K	605.08	Joback Method
cpg	387.30	J/mol×K	640.78	Joback Method
cpg	399.67	J/mol×K	676.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R545712&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume