

2-Carene epoxyde

Other names:	E-2,3-Epoxy-carane
Inchi:	InChI=1S/C10H16O/c1-9(2)6-4-5-10(3)8(11-10)7(6)9/h6-8H,4-5H2,1-3H3/t6-,7-,8?,10?/m
InchiKey:	GGOZBGQCWVKOSB-BGPATTHWSA-N
Formula:	C10H16O
SMILES:	CC12CCC3C(C1O2)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	1153.00		NIST Webbook
rinpol	1191.00		NIST Webbook
rinpol	1153.00		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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R321056&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

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

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