

1,2-Epoxy-5,9-cyclododecadiene

Other names:	13-Oxabicyclo[10.1.0]trideca-4,8-diene
Inchi:	InChI=1S/C12H18O/c1-2-4-6-8-10-12-11(13-12)9-7-5-3-1/h3-6,11-12H,1-2,7-10H2/b5-3+
InchiKey:	OWUVDWLTQIPNLN-GGWOSOGESA-N
Formula:	C12H18O
SMILES:	C1=CCCC2OC2CCC=CCC1
Mol. weight [g/mol]:	178.27
CAS:	943-93-1

Physical Properties

Property code	Value	Unit	Source
gf	60.76	kJ/mol	Joback Method
hf	-204.97	kJ/mol	Joback Method
hfus	18.83	kJ/mol	Joback Method
hvap	48.43	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.220		Crippen Method
mcvol	155.490	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
tb	542.60	K	Joback Method
tc	785.89	K	Joback Method
tf	264.33	K	Joback Method
vc	0.558	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.68	J/molxK	542.60	Joback Method
cpg	409.36	J/molxK	583.15	Joback Method
cpg	431.42	J/molxK	623.70	Joback Method
cpg	451.91	J/molxK	664.25	Joback Method
cpg	470.86	J/molxK	704.79	Joback Method
cpg	488.34	J/molxK	745.34	Joback Method
cpg	504.38	J/molxK	785.89	Joback Method
dvisc	0.0087792	Paxs	264.33	Joback Method

dvisc	0.0029394	Paxs	310.71	Joback Method
dvisc	0.0013077	Paxs	357.09	Joback Method
dvisc	0.0007008	Paxs	403.46	Joback Method
dvisc	0.0004272	Paxs	449.84	Joback Method
dvisc	0.0002856	Paxs	496.22	Joback Method
dvisc	0.0002046	Paxs	542.60	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	356.20	K	0.10	NIST Webbook
tbrp	356.00	K	0.10	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C943931&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
dvisc:	Dynamic viscosity
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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