Ascaridole

Other names:	2,3-Dioxabicyclo[2.2.2]oct-5-ene, 1-methyl-4-(1-methylethyl)-
	p-Menth-2-ene, 1,4-epidioxy-
	Ascaridol
	Ascaricum
	Ascarisin
	Askaridol
	1,4-Peroxido-p-menthene-2
	1,4-Peroxy-p-menth-2-ene
	1,4-Epidioxy-p-menth-2-ene
	2,3-Dioxabicyclo(2.2.2)oct-5-ene, 1-isopropyl-4-methyl-
	1-Methyl-4-(1-methylethyl)-2,3-dioxabicyclo(2.2.2)oct-5-ene
	Ascaridiol
	NSC 406266
	(E)-Ascaridole
	1,4-epidioxy-2-p-menthene
Inchi:	InChI=1S/C10H16O2/c1-8(2)10-6-4-9(3,5-7-10)11-12-10/h4,6,8H,5,7H2,1-3H3
InchiKey:	MGYMHQJELJYRQS-UHFFFAOYSA-N
Formula:	C10H16O2
SMILES:	CC(C)C12C=CC(C)(CC1)OO2
Mol. weight [g/mol]:	168.23
CAS:	512-85-6

Physical Properties

Property code	Value	Unit	Source
gf	-25.08	kJ/mol	Joback Method
hf	-297.47	kJ/mol	Joback Method
hfus	14.79	kJ/mol	Joback Method
hvap	44.65	kJ/mol	Joback Method
ie	8.42	eV	NIST Webbook
ie	8.07	eV	NIST Webbook
log10ws	-2.80		Crippen Method
logp	2.452		Crippen Method
mcvol	137.480	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
rinpol	1257.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1240.00		NIST Webbook

rinpol	1234.00		NIST Webbook
rinpol	1242.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1278.00		NIST Webbook
rinpol	1238.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1278.00		NIST Webbook
rinpol	1238.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1237.00		NIST Webbook
rinpol	1248.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1245.00		NIST Webbook
ripol	1889.00		NIST Webbook
ripol	1860.00		NIST Webbook
ripol	1889.00		NIST Webbook
ripol	1889.00		NIST Webbook
ripol	1860.00		NIST Webbook
tb	503.32	K	Joback Method
tc	731.96	K	Joback Method
tf	276.40	K	NIST Webbook
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.22	J/mol×K	503.32	Joback Method
cpg	354.85	J/mol×K	541.43	Joback Method
cpg	370.88	J/mol×K	579.53	Joback Method
cpg	385.59	J/mol×K	617.64	Joback Method
cpg	399.25	J/mol×K	655.74	Joback Method
cpg	412.14	J/mol×K	693.85	Joback Method
cpg	424.54	J/mol×K	731.96	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source

tbrp	388.20	K	2.00	NIST Webbook
tbrp	312.20	K	0.03	NIST Webbook
tbrp	388.00	K	2.00	NIST Webbook
tbrp	312.50 ± 0.50	K	0.03	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C512856&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
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume