

Fenchol, 2,3-epoxy, exo

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C10H16O2/c1-9(2)5-4-10(3,8(9)11)7-6(5)12-7/h5-8,11H,4H2,1-3H3/t5-,6?,7?,8

ALYCMEVQHFCUJZ-OKEXLJTKSA-N

C10H16O2

CC1(C)C2CC(C)(C3OC23)C1O

168.23

Physical Properties

Property code	Value	Unit	Source
gf	-29.38	kJ/mol	Joback Method
hf	-339.94	kJ/mol	Joback Method
hfus	20.85	kJ/mol	Joback Method
hvap	55.38	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	1.181		Crippen Method
mcvol	130.920	ml/mol	McGowan Method
pc	3306.75	kPa	Joback Method
rinpol	1101.00		NIST Webbook
rinpol	1101.00		NIST Webbook
ripol	1557.00		NIST Webbook
ripol	1557.00		NIST Webbook
tb	549.75	K	Joback Method
tc	749.77	K	Joback Method
tf	382.27	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.40	J/mol×K	549.75	Joback Method
cpg	385.97	J/mol×K	583.09	Joback Method
cpg	399.46	J/mol×K	616.42	Joback Method
cpg	412.08	J/mol×K	649.76	Joback Method
cpg	424.05	J/mol×K	683.09	Joback Method
cpg	435.58	J/mol×K	716.43	Joback Method

Sources

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=R508095&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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