Oxiranecarbonitrile, 3-methyl-3-phenyl-

Other names: 3-methyl-3-phenyl-oxiranecarbonitrile
Inchi: InChI=1S/C10H9NO/c1-10(9(7-11)12-10)8-5-3-2-4-6-8/h2-6,9H,1H3
InchiKey: QCAMDQRKWIVWKA-UHFFFAOYSA-N
Formula: C10H9NO
SMILES: CC1(c2ccccc2)OC1C#N
Mol. weight [g/mol]: 159.18
CAS: 28937-48-6

Physical Properties

Property code	Value	Unit	Source
gf	240.34	kJ/mol	Joback Method
hf	87.38	kJ/mol	Joback Method
hfus	18.09	kJ/mol	Joback Method
hvap	53.57	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	1.824		Crippen Method
mcvol	124.390	ml/mol	McGowan Method
pc	3306.75	kPa	Joback Method
tb	586.22	K	Joback Method
tc	833.84	K	Joback Method
tf	358.04	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.34	J/mol×K	586.22	Joback Method
cpg	313.75	J/mol×K	627.49	Joback Method
cpg	325.17	J/mol×K	668.76	Joback Method
cpg	335.83	J/mol×K	710.03	Joback Method
cpg	345.92	J/mol×K	751.30	Joback Method
cpg	355.66	J/mol×K	792.57	Joback Method
cpg	365.24	J/mol×K	833.84	Joback Method

Sources

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=C28937486&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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