

5,6-Dihydro-2-iso-propenyl-4,4,6-trimethyl-(4H)-1,3-oxazine

Other names:	4H-1,3-Oxazine, 5,6-dihydro-4,4,6-trimethyl-2-(1-methylethenyl)-5,6-dihydro-4,4,6-trimethyl-2-(1-methylvinyl)-4H-1,3-oxazine
Inchi:	InChI=1S/C10H17NO/c1-7(2)9-11-10(4,5)6-8(3)12-9/h8H,1,6H2,2-5H3
InchiKey:	NXCYOVRBLCDPD-UHFFFAOYSA-N
Formula:	C10H17NO
SMILES:	<chem>C=C(C)C1=NC(C)(C)CC(C)O1</chem>
Mol. weight [g/mol]:	167.25
CAS:	39575-65-0

Physical Properties

Property code	Value	Unit	Source
gf	174.85	kJ/mol	Joback Method
hf	-99.59	kJ/mol	Joback Method
hfus	19.62	kJ/mol	Joback Method
hvap	47.91	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.548		Crippen Method
mvol	148.150	ml/mol	McGowan Method
pc	2767.17	kPa	Joback Method
tb	524.67	K	Joback Method
tc	751.24	K	Joback Method
tf	325.17	K	Joback Method
vc	0.564	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.75	J/molxK	524.67	Joback Method
cpg	383.64	J/molxK	562.43	Joback Method
cpg	401.39	J/molxK	600.19	Joback Method
cpg	418.09	J/molxK	637.96	Joback Method
cpg	433.86	J/molxK	675.72	Joback Method
cpg	448.79	J/molxK	713.48	Joback Method
cpg	462.98	J/molxK	751.24	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	352.20	K	2.70	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C39575650&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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