2H-1,3-Oxazine, 2-(4-chlorophenyl)tetrahydro-

Inchi: InChI=1S/C10H12ClNO/c11-9-4-2-8(3-5-9)10-12-6-1-7-13-10/h2-5,10,12H,1,6-7H2
InchiKey: IUSGGJOQPVRUFH-UHFFFAOYSA-N
Formula: C10H12ClNO
SMILES: Clc1ccc(C2NCCCO2)cc1
Mol. weight [g/mol]: 197.66
CAS: 109086-75-1

Physical Properties

Property code	Value	Unit	Source
gf	150.21	kJ/mol	Joback Method
hf	-80.28	kJ/mol	Joback Method
hfus	28.91	kJ/mol	Joback Method
hvap	56.87	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.348		Crippen Method
mcvol	145.230	ml/mol	McGowan Method
pc	3551.53	kPa	Joback Method
tb	592.34	K	Joback Method
tc	849.40	K	Joback Method
tf	410.30	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.72	J/mol×K	592.34	Joback Method
cpg	360.72	J/mol×K	635.18	Joback Method
cpg	376.44	J/mol×K	678.03	Joback Method
cpg	390.93	J/mol×K	720.87	Joback Method
cpg	404.21	J/mol×K	763.71	Joback Method
cpg	416.34	J/mol×K	806.55	Joback Method
cpg	427.35	J/mol×K	849.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C109086751&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
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

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