2-(O-chlorophenyl)benzoxazone-4

Inchi: InChI=1S/C14H10ClNO2/c15-11-7-3-1-5-9(11)14-16-13(17)10-6-2-4-8-12(10)18-14/h1-8
InchiKey: WCWMJTIWVYWUHJ-UHFFFAOYSA-N
Formula: C14H10ClNO2
SMILES: O=C1NC(c2ccccc2Cl)Oc2ccccc21
Mol. weight [g/mol]: 259.69

Physical Properties

Property code	Value	Unit	Source
gf	188.28	kJ/mol	Joback Method
hf	-63.16	kJ/mol	Joback Method
hfus	36.63	kJ/mol	Joback Method
hvap	72.62	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	3.161		Crippen Method
mcvol	179.400	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
tb	774.80	K	Joback Method
tc	1053.97	K	Joback Method
tf	569.58	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.89	J/mol×K	774.80	Joback Method
cpg	496.28	J/mol×K	821.33	Joback Method
cpg	509.18	J/mol×K	867.86	Joback Method
cpg	520.64	J/mol×K	914.39	Joback Method
cpg	530.71	J/mol×K	960.91	Joback Method
cpg	539.44	J/mol×K	1007.44	Joback Method
cpg	546.87	J/mol×K	1053.97	Joback Method

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=B6000034&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume