4-Nitrobenzoic acid, 3-chloroprop-2-enyl ester

Inchi: InChI=1S/C10H8ClNO4/c11-6-1-7-16-10(13)8-2-4-9(5-3-8)12(14)15/h1-6H,7H2/b6-1+
InchiKey: LIVUUKNGTUNKGJ-LZCJLJQNSA-N
Formula: C10H8ClNO4
SMILES: O=C(OCC=CCl)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 241.63

Physical Properties

Property code	Value	Unit	Source
gf	6.02	kJ/mol	Joback Method
hf	-178.75	kJ/mol	Joback Method
hfus	33.85	kJ/mol	Joback Method
hvap	70.88	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	2.504		Crippen Method
mcvol	160.800	ml/mol	McGowan Method
pc	3124.49	kPa	Joback Method
rinpol	1826.00		NIST Webbook
tb	729.58	K	Joback Method
tc	978.90	K	Joback Method
tf	482.01	K	Joback Method
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.58	J/mol×K	729.58	Joback Method
cpg	402.89	J/mol×K	771.13	Joback Method
cpg	412.31	J/mol×K	812.69	Joback Method
cpg	420.89	J/mol×K	854.24	Joback Method
cpg	428.68	J/mol×K	895.80	Joback Method
cpg	435.74	J/mol×K	937.35	Joback Method
cpg	442.12	J/mol×K	978.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299274&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume