2-Chloro-5-nitrobenzyl alcohol, n-butyl ether

Inchi: InChI=1S/C11H14ClNO3/c1-2-3-6-16-8-9-7-10(13(14)15)4-5-11(9)12/h4-5,7H,2-3,6,8H2,
InchiKey: DJVAIFWCYZXKKT-UHFFFAOYSA-N
Formula: C11H14ClNO3
SMILES: CCCCOCc1cc([N+](=O)[O-])ccc1Cl
Mol. weight [g/mol]: 243.69

Physical Properties

Property code	Value	Unit	Source
gf	53.51	kJ/mol	Joback Method
hf	-215.50	kJ/mol	Joback Method
hfus	34.25	kJ/mol	Joback Method
hvap	67.07	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.565		Crippen Method
mcvol	177.620	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
rinpol	1833.00		NIST Webbook
rinpol	1833.00		NIST Webbook
tb	699.41	K	Joback Method
tc	929.90	K	Joback Method
tf	460.95	K	Joback Method
vc	0.693	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.61	J/mol×K	699.41	Joback Method
cpg	468.71	J/mol×K	737.82	Joback Method
cpg	480.91	J/mol×K	776.24	Joback Method
cpg	492.22	J/mol×K	814.65	Joback Method
cpg	502.68	J/mol×K	853.07	Joback Method
cpg	512.31	J/mol×K	891.48	Joback Method
cpg	521.13	J/mol×K	929.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378154&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