2-Chloro-5-nitrobenzyl alcohol, 2-methylpropyl ether

Inchi: InChI=1S/C11H14ClNO3/c1-8(2)6-16-7-9-5-10(13(14)15)3-4-11(9)12/h3-5,8H,6-7H2,1-2

InchiKey: KMOSKQORRIOGTO-UHFFFAOYSA-N

Formula: C11H14ClNO3

SMILES: CC(C)COCc1cc([N+](=O)[O-])ccc1Cl

Mol. weight [g/mol]: 243.69

Physical Properties

Property code	Value	Unit	Source
gf	51.07	kJ/mol	Joback Method
hf	-220.78	kJ/mol	Joback Method
hfus	30.73	kJ/mol	Joback Method
hvap	66.68	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.421		Crippen Method
mcvol	177.620	ml/mol	McGowan Method
pc	2482.59	kPa	Joback Method
rinpol	1780.00		NIST Webbook
rinpol	1780.00		NIST Webbook
tb	698.97	K	Joback Method
tc	933.99	K	Joback Method
tf	445.95	K	Joback Method
vc	0.686	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.18	J/mol×K	698.97	Joback Method
cpg	469.56	J/mol×K	738.14	Joback Method
cpg	481.98	J/mol×K	777.31	Joback Method
cpg	493.49	J/mol×K	816.48	Joback Method
cpg	504.08	J/mol×K	855.65	Joback Method
cpg	513.81	J/mol×K	894.82	Joback Method
cpg	522.67	J/mol×K	933.99	Joback Method

Sources

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=U378151&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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