2-Chloro-5-nitrobenzyl alcohol, 3-methylbutyl ether

Inchi: InChI=1S/C12H16ClNO3/c1-9(2)5-6-17-8-10-7-11(14(15)16)3-4-12(10)13/h3-4,7,9H,5-6,

InchiKey: QYVSKUWQRXVOKJ-UHFFFAOYSA-N

Formula: C12H16ClNO3

SMILES: CC(C)CCOCc1cc([N+](=O)[O-])ccc1Cl

Mol. weight [g/mol]: 257.71

Physical Properties

Property code	Value	Unit	Source
gf	59.49	kJ/mol	Joback Method
hf	-241.42	kJ/mol	Joback Method
hfus	33.32	kJ/mol	Joback Method
hvap	68.90	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	3.811		Crippen Method
mcvol	191.710	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
rinpol	1893.00		NIST Webbook
rinpol	1893.00		NIST Webbook
tb	721.85	K	Joback Method
tc	952.43	K	Joback Method
tf	457.22	K	Joback Method
vc	0.743	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.91	J/mol×K	721.85	Joback Method
cpg	521.80	J/mol×K	760.28	Joback Method
cpg	534.71	J/mol×K	798.71	Joback Method
cpg	546.66	J/mol×K	837.14	Joback Method
cpg	557.69	J/mol×K	875.57	Joback Method
cpg	567.82	J/mol×K	914.00	Joback Method
cpg	577.07	J/mol×K	952.43	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=U378157&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