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

Inchi: InChI=1S/C12H16ClNO3/c1-2-3-4-7-17-9-10-8-11(14(15)16)5-6-12(10)13/h5-6,8H,2-4,7,
InchiKey: XGDSSGLXSAKOFU-UHFFFAOYSA-N
Formula: C12H16ClNO3
SMILES: CCCCCOCc1cc([N+](=O)[O-])ccc1Cl
Mol. weight [g/mol]: 257.71

Physical Properties

Property code	Value	Unit	Source
gf	61.93	kJ/mol	Joback Method
hf	-236.14	kJ/mol	Joback Method
hfus	36.84	kJ/mol	Joback Method
hvap	69.29	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	3.955		Crippen Method
mcvol	191.710	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	1936.00		NIST Webbook
rinpol	1936.00		NIST Webbook
tb	722.29	K	Joback Method
tc	948.64	K	Joback Method
tf	472.22	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.34	J/mol×K	722.29	Joback Method
cpg	520.96	J/mol×K	760.02	Joback Method
cpg	533.65	J/mol×K	797.74	Joback Method
cpg	545.42	J/mol×K	835.47	Joback Method
cpg	556.32	J/mol×K	873.19	Joback Method
cpg	566.36	J/mol×K	910.92	Joback Method
cpg	575.57	J/mol×K	948.64	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=U378158&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume