4-Hydroxy-3-nitrobenzyl alcohol

Inchi:	InChI=1S/C7H7NO4/c9-4-5-1-2-7(10)6(3-5)8(11)12/h1-3,9-10H,4H2
InchiKey:	IMLGJYRKLCMJPI-UHFFFAOYSA-N
Formula:	C7H7NO4
SMILES:	O=[N+]([O-])c1cc(CO)ccc1O
Mol. weight [g/mol]:	169.13
CAS:	41833-13-0

Physical Properties

Property code	Value	Unit	Source
gf	-145.05	kJ/mol	Joback Method
hf	-303.05	kJ/mol	Joback Method
hfus	28.77	kJ/mol	Joback Method
hvap	80.40	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	0.793		Crippen Method
mcvol	114.890	ml/mol	McGowan Method
pc	5730.52	kPa	Joback Method
tb	715.86	K	Joback Method
tc	951.77	K	Joback Method
tf	523.74	K	Joback Method
vc	0.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.26	J/mol×K	715.86	Joback Method
cpg	306.76	J/mol×K	755.18	Joback Method
cpg	313.80	J/mol×K	794.50	Joback Method
cpg	320.44	J/mol×K	833.81	Joback Method
cpg	326.79	J/mol×K	873.13	Joback Method
cpg	332.91	J/mol×K	912.45	Joback Method
cpg	338.91	J/mol×K	951.77	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=C41833130&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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