3-Nitrobenzyl alcohol, pentafluoropropionate

Inchi: InChI=1S/C10H6F5NO4/c11-9(12,10(13,14)15)8(17)20-5-6-2-1-3-7(4-6)16(18)19/h1-4H,
InchiKey: BIGJTYYYNLMSSD-UHFFFAOYSA-N
Formula: C10H6F5NO4
SMILES: O=C(OCc1cccc([N+](=O)[O-])c1)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 299.15

Physical Properties

Property code	Value	Unit	Source
gf	-1030.64	kJ/mol	Joback Method
hf	-1278.28	kJ/mol	Joback Method
hfus	30.03	kJ/mol	Joback Method
hvap	59.86	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	2.836		Crippen Method
mcvol	161.710	ml/mol	McGowan Method
pc	2522.65	kPa	Joback Method
rinpol	1423.00		NIST Webbook
tb	677.88	K	Joback Method
tc	889.99	K	Joback Method
tf	464.96	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.87	J/mol×K	677.88	Joback Method
cpg	451.85	J/mol×K	713.23	Joback Method
cpg	460.96	J/mol×K	748.58	Joback Method
cpg	469.24	J/mol×K	783.93	Joback Method
cpg	476.77	J/mol×K	819.28	Joback Method
cpg	483.59	J/mol×K	854.63	Joback Method
cpg	489.79	J/mol×K	889.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376154&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