2-Methyl-3-nitrobenzyl alcohol, pentafluoropropionate

Inchi: InChI=1S/C11H8F5NO4/c1-6-7(3-2-4-8(6)17(19)20)5-21-9(18)10(12,13)11(14,15)16/h2-4

InchiKey: KOLZDRJTMNZCEM-UHFFFAOYSA-N

Formula: C11H8F5NO4

SMILES: Cc1c(COC(=O)C(F)(F)C(F)(F)F)cccc1[N+](=O)[O-]

Mol. weight [g/mol]: 313.18

Physical Properties

Property code	Value	Unit	Source
gf	-1031.85	kJ/mol	Joback Method
hf	-1310.39	kJ/mol	Joback Method
hfus	32.23	kJ/mol	Joback Method
hvap	62.75	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.144		Crippen Method
mcvol	175.800	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
rinpol	1473.00		NIST Webbook
rinpol	1473.00		NIST Webbook
tb	705.74	K	Joback Method
tc	915.65	K	Joback Method
tf	488.75	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.00	J/mol×K	705.74	Joback Method
cpg	500.36	J/mol×K	740.72	Joback Method
cpg	509.86	J/mol×K	775.71	Joback Method
cpg	518.57	J/mol×K	810.69	Joback Method
cpg	526.53	J/mol×K	845.68	Joback Method
cpg	533.81	J/mol×K	880.66	Joback Method
cpg	540.46	J/mol×K	915.65	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=U376201&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