3-Nitrobenzyl alcohol, heptafluorobutyrate

Inchi: InChI=1S/C11H6F7NO4/c12-9(13,10(14,15)11(16,17)18)8(20)23-5-6-2-1-3-7(4-6)19(21)2
InchiKey: HWXCMQNJHLYUJP-UHFFFAOYSA-N
Formula: C11H6F7NO4
SMILES: O=C(OCc1cccc([N+](=O)[O-])c1)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 349.16

Physical Properties

Property code	Value	Unit	Source
gf	-1409.00	kJ/mol	Joback Method
hf	-1699.89	kJ/mol	Joback Method
hfus	31.36	kJ/mol	Joback Method
hvap	59.16	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	3.471		Crippen Method
mcvol	179.340	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
rinpol	1458.00		NIST Webbook
rinpol	1458.00		NIST Webbook
tb	696.07	K	Joback Method
tc	898.84	K	Joback Method
tf	479.83	K	Joback Method
vc	0.743	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.59	J/mol×K	696.07	Joback Method
cpg	520.39	J/mol×K	729.86	Joback Method
cpg	529.29	J/mol×K	763.66	Joback Method
cpg	537.37	J/mol×K	797.45	Joback Method
cpg	544.71	J/mol×K	831.25	Joback Method
cpg	551.38	J/mol×K	865.04	Joback Method
cpg	557.47	J/mol×K	898.84	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=U376153&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