2-Methyl-3-nitrobenzyl alcohol, heptafluorobutyrate

Inchi: InChI=1S/C12H8F7NO4/c1-6-7(3-2-4-8(6)20(22)23)5-24-9(21)10(13,14)11(15,16)12(17,1

InchiKey: JGHFWASYXRGMGP-UHFFFAOYSA-N

Formula: C12H8F7NO4

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

Mol. weight [g/mol]: 363.19

Physical Properties

Property code	Value	Unit	Source
gf	-1410.21	kJ/mol	Joback Method
hf	-1732.00	kJ/mol	Joback Method
hfus	33.56	kJ/mol	Joback Method
hvap	62.05	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	3.779		Crippen Method
mcvol	193.430	ml/mol	McGowan Method
pc	1942.37	kPa	Joback Method
rinpol	1508.00		NIST Webbook
tb	723.93	K	Joback Method
tc	925.36	K	Joback Method
tf	503.62	K	Joback Method
vc	0.798	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.53	J/mol×K	723.93	Joback Method
cpg	569.63	J/mol×K	757.50	Joback Method
cpg	578.87	J/mol×K	791.07	Joback Method
cpg	587.32	J/mol×K	824.65	Joback Method
cpg	595.05	J/mol×K	858.22	Joback Method
cpg	602.14	J/mol×K	891.79	Joback Method
cpg	608.66	J/mol×K	925.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376200&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

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