4-Bromobenzyl alcohol, heptafluorobutyrate

Inchi: InChI=1S/C11H6BrF7O2/c12-7-3-1-6(2-4-7)5-21-8(20)9(13,14)10(15,16)11(17,18)19/h1-
InchiKey: MMOYUTURYPJAGV-UHFFFAOYSA-N
Formula: C11H6BrF7O2
SMILES: O=C(OCc1ccc(Br)cc1)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 383.06

Physical Properties

Property code	Value	Unit	Source
gf	-1430.23	kJ/mol	Joback Method
hf	-1662.80	kJ/mol	Joback Method
hfus	25.29	kJ/mol	Joback Method
hvap	49.00	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.325		Crippen Method
mcvol	179.420	ml/mol	McGowan Method
pc	2265.42	kPa	Joback Method
rinpol	1319.00		NIST Webbook
rinpol	1319.00		NIST Webbook
tb	610.39	K	Joback Method
tc	802.12	K	Joback Method
tf	396.02	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.44	J/mol×K	610.39	Joback Method
cpg	463.07	J/mol×K	642.35	Joback Method
cpg	472.79	J/mol×K	674.30	Joback Method
cpg	481.68	J/mol×K	706.26	Joback Method
cpg	489.79	J/mol×K	738.21	Joback Method
cpg	497.19	J/mol×K	770.17	Joback Method
cpg	503.96	J/mol×K	802.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376144&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