4-Bromobenzyl alcohol, pentafluoropropionate

Inchi: InChI=1S/C10H6BrF5O2/c11-7-3-1-6(2-4-7)5-18-8(17)9(12,13)10(14,15)16/h1-4H,5H2
InchiKey: QKXWGASKQLFKSW-UHFFFAOYSA-N
Formula: C10H6BrF5O2
SMILES: O=C(OCc1ccc(Br)cc1)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 333.05

Physical Properties

Property code	Value	Unit	Source
gf	-1051.87	kJ/mol	Joback Method
hf	-1241.19	kJ/mol	Joback Method
hfus	23.95	kJ/mol	Joback Method
hvap	49.71	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	3.690		Crippen Method
mcvol	161.790	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
rinpol	1281.00		NIST Webbook
tb	592.20	K	Joback Method
tc	793.33	K	Joback Method
tf	381.15	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.52	J/mol×K	592.20	Joback Method
cpg	396.06	J/mol×K	625.72	Joback Method
cpg	405.74	J/mol×K	659.24	Joback Method
cpg	414.63	J/mol×K	692.76	Joback Method
cpg	422.77	J/mol×K	726.29	Joback Method
cpg	430.22	J/mol×K	759.81	Joback Method
cpg	437.04	J/mol×K	793.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376145&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

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