Benzyl alcohol, heptafluorobutyrate

Other names: Benzenemethanol, heptafluorobutanoate
Inchi: InChI=1S/C11H7F7O2/c12-9(13,10(14,15)11(16,17)18)8(19)20-6-7-4-2-1-3-5-7/h1-5H,6
InchiKey: OGKFEKRYHDUTNO-UHFFFAOYSA-N
Formula: C11H7F7O2
SMILES: O=C(OCc1ccccc1)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 304.16

Physical Properties

Property code	Value	Unit	Source
gf	-1434.92	kJ/mol	Joback Method
hf	-1677.66	kJ/mol	Joback Method
hfus	20.39	kJ/mol	Joback Method
hvap	41.91	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.563		Crippen Method
mcvol	161.920	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
rinpol	1060.00		NIST Webbook
rinpol	1060.00		NIST Webbook
tb	539.25	K	Joback Method
tc	717.64	K	Joback Method
tf	323.70	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.98	J/mol×K	539.25	Joback Method
cpg	426.54	J/mol×K	568.98	Joback Method
cpg	438.16	J/mol×K	598.71	Joback Method
cpg	448.89	J/mol×K	628.44	Joback Method
cpg	458.79	J/mol×K	658.18	Joback Method
cpg	467.91	J/mol×K	687.91	Joback Method
cpg	476.29	J/mol×K	717.64	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=U365382&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