4-Hydroxyphenethyl alcohol, bis(heptafluorobutyrate)

Inchi: InChI=1S/C16H8F14O4/c17-11(18,13(21,22)15(25,26)27)9(31)33-6-5-7-1-3-8(4-2-7)34-1

InchiKey: LTRMDJZKFVUVMX-UHFFFAOYSA-N

Formula: C16H8F14O4

SMILES: O=C(OCCc1ccc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)cc1)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 530.21

Physical Properties

Property code	Value	Unit	Source
gf	-2991.52	kJ/mol	Joback Method
hf	-3436.15	kJ/mol	Joback Method
hfus	35.06	kJ/mol	Joback Method
hvap	53.25	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	5.344		Crippen Method
mcvol	252.200	ml/mol	McGowan Method
pc	1220.85	kPa	Joback Method
rinpol	1390.00		NIST Webbook
tb	720.12	K	Joback Method
tc	888.26	K	Joback Method
tf	476.12	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	772.02	J/mol×K	720.12	Joback Method
cpg	782.43	J/mol×K	748.14	Joback Method
cpg	791.98	J/mol×K	776.17	Joback Method
cpg	800.73	J/mol×K	804.19	Joback Method
cpg	808.77	J/mol×K	832.21	Joback Method
cpg	816.17	J/mol×K	860.24	Joback Method
cpg	823.00	J/mol×K	888.26	Joback Method

Sources

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=U376197&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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