3-Hydroxybenzyl alcohol, bis(heptafluorobutyrate)

Inchi: InChI=1S/C15H6F14O4/c16-10(17,12(20,21)14(24,25)26)8(30)32-5-6-2-1-3-7(4-6)33-9(3

InchiKey: SWKUBRXBUQUXDF-UHFFFAOYSA-N

Formula: C15H6F14O4

SMILES: O=C(OCc1cccc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 516.18

Physical Properties

Property code	Value	Unit	Source
gf	-2999.94	kJ/mol	Joback Method
hf	-3415.51	kJ/mol	Joback Method
hfus	32.47	kJ/mol	Joback Method
hvap	51.02	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	5.301		Crippen Method
mcvol	238.110	ml/mol	McGowan Method
pc	1307.06	kPa	Joback Method
rinpol	1263.00		NIST Webbook
rinpol	1263.00		NIST Webbook
tb	697.24	K	Joback Method
tc	863.56	K	Joback Method
tf	464.85	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.91	J/mol×K	697.24	Joback Method
cpg	729.98	J/mol×K	724.96	Joback Method
cpg	739.18	J/mol×K	752.68	Joback Method
cpg	747.59	J/mol×K	780.40	Joback Method
cpg	755.28	J/mol×K	808.12	Joback Method
cpg	762.32	J/mol×K	835.84	Joback Method
cpg	768.78	J/mol×K	863.56	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376159&Units=SI

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