2-Amino-1-phenylethanol, N,O-bis(heptafluorobutyryl)-

Inchi: InChI=1S/C16H9F14NO3/c17-11(18,13(21,22)15(25,26)27)9(32)31-6-8(7-4-2-1-3-5-7)34
InchiKey: NXKYNDOXUWFJJJ-UHFFFAOYSA-N
Formula: C16H9F14NO3
SMILES: O=C(NCC(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1ccccc1)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 529.23
CAS: 959257-87-5

Physical Properties

Property code	Value	Unit	Source
gf	-2789.94	kJ/mol	Joback Method
hf	-3244.27	kJ/mol	Joback Method
hfus	35.83	kJ/mol	Joback Method
hvap	56.22	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	5.053		Crippen Method
mcvol	256.310	ml/mol	McGowan Method
pc	1267.35	kPa	Joback Method
rinpol	1381.00		NIST Webbook
rinpol	1381.00		NIST Webbook
tb	742.45	K	Joback Method
tc	915.10	K	Joback Method
tf	479.03	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	799.76	J/mol×K	742.45	Joback Method
cpg	810.05	J/mol×K	771.23	Joback Method
cpg	819.45	J/mol×K	800.00	Joback Method
cpg	828.05	J/mol×K	828.78	Joback Method
cpg	835.96	J/mol×K	857.55	Joback Method
cpg	843.27	J/mol×K	886.33	Joback Method
cpg	850.06	J/mol×K	915.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C959257875&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

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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