4-Aminobenzoic acid, N,O-bis(heptafluorobutyryl)-

Inchi: InChI=1S/C15H5F14NO4/c16-10(17,12(20,21)14(24,25)26)8(32)30-6-3-1-5(2-4-6)7(31)3
InchiKey: RYLLEUUQVWFZLM-UHFFFAOYSA-N
Formula: C15H5F14NO4
SMILES: O=C(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1ccc(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)cc1
Mol. weight [g/mol]: 529.18

Physical Properties

Property code	Value	Unit	Source
gf	-2934.47	kJ/mol	Joback Method
hf	-3342.40	kJ/mol	Joback Method
hfus	37.98	kJ/mol	Joback Method
hvap	61.79	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	4.974		Crippen Method
mcvol	243.790	ml/mol	McGowan Method
pc	1399.59	kPa	Joback Method
rinpol	1537.00		NIST Webbook
rinpol	1537.00		NIST Webbook
tb	778.86	K	Joback Method
tc	958.53	K	Joback Method
tf	545.21	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.67	J/mol×K	778.86	Joback Method
cpg	763.81	J/mol×K	808.81	Joback Method
cpg	771.19	J/mol×K	838.75	Joback Method
cpg	777.89	J/mol×K	868.70	Joback Method
cpg	784.03	J/mol×K	898.64	Joback Method
cpg	789.70	J/mol×K	928.59	Joback Method
cpg	794.98	J/mol×K	958.53	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=U375075&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