Benzoic acid, 4-(heptafluorobutyrylamino)-

Inchi: InChI=1S/C11H6F7NO3/c12-9(13,10(14,15)11(16,17)18)8(22)19-6-3-1-5(2-4-6)7(20)21/h
InchiKey: QCHWYLKDUSWZMO-UHFFFAOYSA-N
Formula: C11H6F7NO3
SMILES: O=C(O)c1ccc(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)cc1
Mol. weight [g/mol]: 333.16

Physical Properties

Property code	Value	Unit	Source
gf	-1515.90	kJ/mol	Joback Method
hf	-1768.25	kJ/mol	Joback Method
hfus	29.60	kJ/mol	Joback Method
hvap	70.02	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.156		Crippen Method
mcvol	173.470	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
rinpol	1773.00		NIST Webbook
rinpol	1773.00		NIST Webbook
tb	718.03	K	Joback Method
tc	901.87	K	Joback Method
tf	477.40	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.80	J/mol×K	718.03	Joback Method
cpg	507.71	J/mol×K	748.67	Joback Method
cpg	514.93	J/mol×K	779.31	Joback Method
cpg	521.54	J/mol×K	809.95	Joback Method
cpg	527.60	J/mol×K	840.59	Joback Method
cpg	533.18	J/mol×K	871.23	Joback Method
cpg	538.33	J/mol×K	901.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375122&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