Benzamide, pentafluoro-N-(3-methylbutyl)-

Inchi: InChI=1S/C12H12F5NO/c1-5(2)3-4-18-12(19)6-7(13)9(15)11(17)10(16)8(6)14/h5H,3-4H2
InchiKey: OAOMPSPVLQFKQN-UHFFFAOYSA-N
Formula: C12H12F5NO
SMILES: CC(C)CCNC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 281.22

Physical Properties

Property code	Value	Unit	Source
gf	-901.60	kJ/mol	Joback Method
hf	-1156.77	kJ/mol	Joback Method
hfus	37.51	kJ/mol	Joback Method
hvap	56.60	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	3.158		Crippen Method
mcvol	176.580	ml/mol	McGowan Method
pc	1966.56	kPa	Joback Method
rinpol	1570.00		NIST Webbook
rinpol	1570.00		NIST Webbook
tb	625.49	K	Joback Method
tc	801.69	K	Joback Method
tf	404.56	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.14	J/mol×K	625.49	Joback Method
cpg	469.68	J/mol×K	654.86	Joback Method
cpg	480.66	J/mol×K	684.22	Joback Method
cpg	491.10	J/mol×K	713.59	Joback Method
cpg	501.01	J/mol×K	742.96	Joback Method
cpg	510.40	J/mol×K	772.33	Joback Method
cpg	519.28	J/mol×K	801.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407938&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