Benzamide, pentafluoro-N-pentyl-

Inchi: InChI=1S/C12H12F5NO/c1-2-3-4-5-18-12(19)6-7(13)9(15)11(17)10(16)8(6)14/h2-5H2,1H
InchiKey: COYUSQTUAZYIPZ-UHFFFAOYSA-N
Formula: C12H12F5NO
SMILES: CCCCCNC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 281.22

Physical Properties

Property code	Value	Unit	Source
gf	-899.16	kJ/mol	Joback Method
hf	-1151.49	kJ/mol	Joback Method
hfus	41.03	kJ/mol	Joback Method
hvap	56.99	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	3.302		Crippen Method
mcvol	176.580	ml/mol	McGowan Method
pc	1952.68	kPa	Joback Method
rinpol	1607.00		NIST Webbook
rinpol	1607.00		NIST Webbook
tb	625.93	K	Joback Method
tc	799.45	K	Joback Method
tf	419.56	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.67	J/mol×K	625.93	Joback Method
cpg	468.99	J/mol×K	654.85	Joback Method
cpg	479.78	J/mol×K	683.77	Joback Method
cpg	490.06	J/mol×K	712.69	Joback Method
cpg	499.83	J/mol×K	741.61	Joback Method
cpg	509.09	J/mol×K	770.53	Joback Method
cpg	517.87	J/mol×K	799.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407939&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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