Benzamide, pentafluoro-N-(2-ethylhexyl)-

Inchi: InChI=1S/C15H18F5NO/c1-3-5-6-8(4-2)7-21-15(22)9-10(16)12(18)14(20)13(19)11(9)17/
InchiKey: KIPJFMIOOGOLNP-UHFFFAOYSA-N
Formula: C15H18F5NO
SMILES: CCCCC(CC)CNC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 323.30

Physical Properties

Property code	Value	Unit	Source
gf	-876.34	kJ/mol	Joback Method
hf	-1218.69	kJ/mol	Joback Method
hfus	45.28	kJ/mol	Joback Method
hvap	63.28	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	4.328		Crippen Method
mcvol	218.850	ml/mol	McGowan Method
pc	1546.35	kPa	Joback Method
rinpol	1802.00		NIST Webbook
rinpol	1802.00		NIST Webbook
tb	694.13	K	Joback Method
tc	869.09	K	Joback Method
tf	438.37	K	Joback Method
vc	0.892	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	612.65	J/mol×K	694.13	Joback Method
cpg	625.97	J/mol×K	723.29	Joback Method
cpg	638.63	J/mol×K	752.45	Joback Method
cpg	650.64	J/mol×K	781.61	Joback Method
cpg	662.01	J/mol×K	810.77	Joback Method
cpg	672.75	J/mol×K	839.93	Joback Method
cpg	682.89	J/mol×K	869.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407942&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