Benzamide, pentafluoro-N-octyl-

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

Physical Properties

Property code	Value	Unit	Source
gf	-873.90	kJ/mol	Joback Method
hf	-1213.41	kJ/mol	Joback Method
hfus	48.80	kJ/mol	Joback Method
hvap	63.67	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	4.472		Crippen Method
mcvol	218.850	ml/mol	McGowan Method
pc	1536.66	kPa	Joback Method
rinpol	1896.00		NIST Webbook
rinpol	1896.00		NIST Webbook
tb	694.57	K	Joback Method
tc	867.56	K	Joback Method
tf	453.37	K	Joback Method
vc	0.898	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	612.14	J/mol×K	694.57	Joback Method
cpg	625.29	J/mol×K	723.40	Joback Method
cpg	637.79	J/mol×K	752.23	Joback Method
cpg	649.67	J/mol×K	781.07	Joback Method
cpg	660.93	J/mol×K	809.90	Joback Method
cpg	671.58	J/mol×K	838.73	Joback Method
cpg	681.65	J/mol×K	867.56	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=U407944&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