Benzamide, pentafluoro-N-decyl-

Inchi: InChI=1S/C17H22F5NO/c1-2-3-4-5-6-7-8-9-10-23-17(24)11-12(18)14(20)16(22)15(21)13
InchiKey: WYKJFCHNTXJVFF-UHFFFAOYSA-N
Formula: C17H22F5NO
SMILES: CCCCCCCCCCNC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 351.35

Physical Properties

Property code	Value	Unit	Source
gf	-857.06	kJ/mol	Joback Method
hf	-1254.69	kJ/mol	Joback Method
hfus	53.98	kJ/mol	Joback Method
hvap	68.12	kJ/mol	Joback Method
log10ws	-7.24		Crippen Method
logp	5.253		Crippen Method
mcvol	247.030	ml/mol	McGowan Method
pc	1329.07	kPa	Joback Method
rinpol	2096.00		NIST Webbook
rinpol	2096.00		NIST Webbook
tb	740.33	K	Joback Method
tc	915.35	K	Joback Method
tf	475.91	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.58	J/mol×K	740.33	Joback Method
cpg	735.79	J/mol×K	769.50	Joback Method
cpg	749.27	J/mol×K	798.67	Joback Method
cpg	762.04	J/mol×K	827.84	Joback Method
cpg	774.12	J/mol×K	857.01	Joback Method
cpg	785.52	J/mol×K	886.18	Joback Method
cpg	796.27	J/mol×K	915.35	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=U407946&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