Benzamide, 2,3,4-trifluoro-N-pentyl-

Inchi: InChI=1S/C12H14F3NO/c1-2-3-4-7-16-12(17)8-5-6-9(13)11(15)10(8)14/h5-6H,2-4,7H2,1
InchiKey: IQJCNZVUXLLPNS-UHFFFAOYSA-N
Formula: C12H14F3NO
SMILES: CCCCCNC(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 245.24

Physical Properties

Property code	Value	Unit	Source
gf	-490.28	kJ/mol	Joback Method
hf	-736.33	kJ/mol	Joback Method
hfus	35.65	kJ/mol	Joback Method
hvap	57.30	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.024		Crippen Method
mcvol	173.040	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	1622.00		NIST Webbook
rinpol	1622.00		NIST Webbook
tb	617.43	K	Joback Method
tc	802.79	K	Joback Method
tf	393.34	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.84	J/mol×K	617.43	Joback Method
cpg	455.50	J/mol×K	648.32	Joback Method
cpg	467.51	J/mol×K	679.22	Joback Method
cpg	478.88	J/mol×K	710.11	Joback Method
cpg	489.63	J/mol×K	741.00	Joback Method
cpg	499.78	J/mol×K	771.89	Joback Method
cpg	509.35	J/mol×K	802.79	Joback Method

Sources

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=U407262&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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