Benzamide, 2-fluoro-3-trifluoromethyl-N-pentyl-N-butyl-

Inchi: InChI=1S/C17H23F4NO/c1-3-5-7-12-22(11-6-4-2)16(23)13-9-8-10-14(15(13)18)17(19,20

InchiKey: QLMRJELCFMANJF-UHFFFAOYSA-N

Formula: C17H23F4NO

SMILES: CCCCCN(CCCC)C(=O)c1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 333.36

Physical Properties

Property code	Value	Unit	Source
gf	-609.13	kJ/mol	Joback Method
hf	-1018.86	kJ/mol	Joback Method
hfus	42.57	kJ/mol	Joback Method
hvap	61.26	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	5.277		Crippen Method
mcvol	245.260	ml/mol	McGowan Method
pc	1425.07	kPa	Joback Method
rinpol	2135.00		NIST Webbook
rinpol	2135.00		NIST Webbook
tb	685.16	K	Joback Method
tc	862.10	K	Joback Method
tf	419.99	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.40	J/mol×K	685.16	Joback Method
cpg	715.16	J/mol×K	714.65	Joback Method
cpg	730.03	J/mol×K	744.14	Joback Method
cpg	744.06	J/mol×K	773.63	Joback Method
cpg	757.30	J/mol×K	803.12	Joback Method
cpg	769.78	J/mol×K	832.61	Joback Method
cpg	781.56	J/mol×K	862.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415528&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