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

Inchi: InChI=1S/C18H25F4NO/c1-3-5-7-12-23(13-8-6-4-2)17(24)14-10-9-11-15(16(14)19)18(20

InchiKey: ACWHJPUSCDJFGN-UHFFFAOYSA-N

Formula: C18H25F4NO

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

Mol. weight [g/mol]: 347.39

Physical Properties

Property code	Value	Unit	Source
gf	-600.71	kJ/mol	Joback Method
hf	-1039.50	kJ/mol	Joback Method
hfus	45.16	kJ/mol	Joback Method
hvap	63.49	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.667		Crippen Method
mcvol	259.350	ml/mol	McGowan Method
pc	1327.14	kPa	Joback Method
rinpol	2591.00		NIST Webbook
rinpol	2591.00		NIST Webbook
tb	708.04	K	Joback Method
tc	885.04	K	Joback Method
tf	431.26	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.01	J/mol×K	708.04	Joback Method
cpg	771.12	J/mol×K	737.54	Joback Method
cpg	786.32	J/mol×K	767.04	Joback Method
cpg	800.67	J/mol×K	796.54	Joback Method
cpg	814.22	J/mol×K	826.04	Joback Method
cpg	827.00	J/mol×K	855.54	Joback Method
cpg	839.07	J/mol×K	885.04	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415530&Units=SI

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