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

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

InchiKey: ZPZBOJDBMAYOIE-UHFFFAOYSA-N

Formula: C18H25F4NO

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

Mol. weight [g/mol]: 347.39

Physical Properties

Property code	Value	Unit	Source
gf	-603.15	kJ/mol	Joback Method
hf	-1044.78	kJ/mol	Joback Method
hfus	41.64	kJ/mol	Joback Method
hvap	63.10	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.523		Crippen Method
mcvol	259.350	ml/mol	McGowan Method
pc	1334.91	kPa	Joback Method
rinpol	2309.00		NIST Webbook
rinpol	2309.00		NIST Webbook
tb	707.60	K	Joback Method
tc	886.64	K	Joback Method
tf	416.26	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.49	J/mol×K	707.60	Joback Method
cpg	771.81	J/mol×K	737.44	Joback Method
cpg	787.19	J/mol×K	767.28	Joback Method
cpg	801.70	J/mol×K	797.12	Joback Method
cpg	815.37	J/mol×K	826.96	Joback Method
cpg	828.26	J/mol×K	856.80	Joback Method
cpg	840.41	J/mol×K	886.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415529&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