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

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

InchiKey: GSLFJWRZPUZUOO-UHFFFAOYSA-N

Formula: C17H23F4NO

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

Mol. weight [g/mol]: 333.36

Physical Properties

Property code	Value	Unit	Source
gf	-611.57	kJ/mol	Joback Method
hf	-1024.14	kJ/mol	Joback Method
hfus	39.05	kJ/mol	Joback Method
hvap	60.87	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	5.133		Crippen Method
mcvol	245.260	ml/mol	McGowan Method
pc	1433.72	kPa	Joback Method
rinpol	2064.00		NIST Webbook
rinpol	2064.00		NIST Webbook
tb	684.72	K	Joback Method
tc	863.96	K	Joback Method
tf	404.99	K	Joback Method
vc	0.959	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.87	J/mol×K	684.72	Joback Method
cpg	715.86	J/mol×K	714.59	Joback Method
cpg	730.94	J/mol×K	744.47	Joback Method
cpg	745.14	J/mol×K	774.34	Joback Method
cpg	758.52	J/mol×K	804.22	Joback Method
cpg	771.13	J/mol×K	834.09	Joback Method
cpg	783.00	J/mol×K	863.96	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=U415527&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