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

Inchi: InChI=1S/C16H21F4NO/c1-3-5-6-11-21(10-4-2)15(22)12-8-7-9-13(14(12)17)16(18,19)20

InchiKey: SOQLAEMPULHZPZ-UHFFFAOYSA-N

Formula: C16H21F4NO

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

Mol. weight [g/mol]: 319.34

Physical Properties

Property code	Value	Unit	Source
gf	-617.55	kJ/mol	Joback Method
hf	-998.22	kJ/mol	Joback Method
hfus	39.98	kJ/mol	Joback Method
hvap	59.03	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	4.887		Crippen Method
mcvol	231.170	ml/mol	McGowan Method
pc	1534.26	kPa	Joback Method
rinpol	1997.00		NIST Webbook
rinpol	1997.00		NIST Webbook
tb	662.28	K	Joback Method
tc	839.62	K	Joback Method
tf	408.72	K	Joback Method
vc	0.908	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.93	J/mol×K	662.28	Joback Method
cpg	660.33	J/mol×K	691.84	Joback Method
cpg	674.86	J/mol×K	721.39	Joback Method
cpg	688.55	J/mol×K	750.95	Joback Method
cpg	701.46	J/mol×K	780.51	Joback Method
cpg	713.63	J/mol×K	810.07	Joback Method
cpg	725.10	J/mol×K	839.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415526&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