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

Inchi: InChI=1S/C22H33F4NO/c1-3-5-7-8-9-10-12-17-27(16-11-6-4-2)21(28)18-14-13-15-19(20

InchiKey: IFFVBYLODBEZDK-UHFFFAOYSA-N

Formula: C22H33F4NO

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

Mol. weight [g/mol]: 403.50

Physical Properties

Property code	Value	Unit	Source
gf	-567.03	kJ/mol	Joback Method
hf	-1122.06	kJ/mol	Joback Method
hfus	55.52	kJ/mol	Joback Method
hvap	72.39	kJ/mol	Joback Method
log10ws	-8.07		Crippen Method
logp	7.228		Crippen Method
mcvol	315.710	ml/mol	McGowan Method
pc	1021.38	kPa	Joback Method
rinpol	2882.00		NIST Webbook
rinpol	2882.00		NIST Webbook
tb	799.56	K	Joback Method
tc	982.39	K	Joback Method
tf	476.34	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	987.51	J/mol×K	799.56	Joback Method
cpg	1005.07	J/mol×K	830.03	Joback Method
cpg	1021.64	J/mol×K	860.50	Joback Method
cpg	1037.28	J/mol×K	890.98	Joback Method
cpg	1052.05	J/mol×K	921.45	Joback Method
cpg	1066.01	J/mol×K	951.92	Joback Method
cpg	1079.21	J/mol×K	982.39	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=U416697&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

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