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

Inchi: InChI=1S/C20H29F4NO/c1-4-6-8-11-15(3)25(14-9-7-5-2)19(26)16-12-10-13-17(18(16)21

InchiKey: NIVNXVKDDGAZJT-UHFFFAOYSA-N

Formula: C20H29F4NO

SMILES: CCCCCC(C)N(CCCCC)C(=O)c1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 375.44

Physical Properties

Property code	Value	Unit	Source
gf	-586.31	kJ/mol	Joback Method
hf	-1086.06	kJ/mol	Joback Method
hfus	46.82	kJ/mol	Joback Method
hvap	67.55	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	6.446		Crippen Method
mcvol	287.530	ml/mol	McGowan Method
pc	1165.63	kPa	Joback Method
rinpol	2694.00		NIST Webbook
rinpol	2694.00		NIST Webbook
tb	753.36	K	Joback Method
tc	933.55	K	Joback Method
tf	438.80	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	869.87	J/mol×K	753.36	Joback Method
cpg	886.83	J/mol×K	783.39	Joback Method
cpg	902.82	J/mol×K	813.42	Joback Method
cpg	917.90	J/mol×K	843.45	Joback Method
cpg	932.13	J/mol×K	873.49	Joback Method
cpg	945.56	J/mol×K	903.52	Joback Method
cpg	958.23	J/mol×K	933.55	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=U415531&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