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

Inchi: InChI=1S/C19H27F4NO/c1-3-5-7-9-14-24(13-8-6-4-2)18(25)15-11-10-12-16(17(15)20)19

InchiKey: GWUGYDOCVWTPJX-UHFFFAOYSA-N

Formula: C19H27F4NO

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

Mol. weight [g/mol]: 361.42

Physical Properties

Property code	Value	Unit	Source
gf	-592.29	kJ/mol	Joback Method
hf	-1060.14	kJ/mol	Joback Method
hfus	47.75	kJ/mol	Joback Method
hvap	65.71	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	6.057		Crippen Method
mcvol	273.440	ml/mol	McGowan Method
pc	1238.96	kPa	Joback Method
rinpol	2423.00		NIST Webbook
rinpol	2423.00		NIST Webbook
tb	730.92	K	Joback Method
tc	908.48	K	Joback Method
tf	442.53	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	811.69	J/mol×K	730.92	Joback Method
cpg	828.14	J/mol×K	760.51	Joback Method
cpg	843.67	J/mol×K	790.11	Joback Method
cpg	858.34	J/mol×K	819.70	Joback Method
cpg	872.18	J/mol×K	849.29	Joback Method
cpg	885.25	J/mol×K	878.89	Joback Method
cpg	897.60	J/mol×K	908.48	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=U416693&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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