

3-Fluoro-6-trifluoromethylbenzamide, N,N-dihexyl-

Inchi:	InChI=1S/C20H29F4NO/c1-3-5-7-9-13-25(14-10-8-6-4-2)19(26)17-15-16(21)11-12-18(17)
InchiKey:	VMLMLVHFAUXQSU-UHFFFAOYSA-N
Formula:	C20H29F4NO
SMILES:	CCCCCN(CCCCC)C(=O)c1cc(F)ccc1C(F)(F)F
Mol. weight [g/mol]:	375.44

Physical Properties

Property code	Value	Unit	Source
gf	-583.87	kJ/mol	Joback Method
hf	-1080.78	kJ/mol	Joback Method
hfus	50.34	kJ/mol	Joback Method
hvap	67.94	kJ/mol	Joback Method
log10ws	-7.24		Crippen Method
logp	6.447		Crippen Method
mcvol	287.530	ml/mol	McGowan Method
pc	1159.29	kPa	Joback Method
rinpol	2107.00		NIST Webbook
rinpol	2107.00		NIST Webbook
tb	753.80	K	Joback Method
tc	932.48	K	Joback Method
tf	453.80	K	Joback Method
vc	1.133	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	869.38	J/mol×K	753.80	Joback Method
cpg	886.18	J/mol×K	783.58	Joback Method
cpg	902.04	J/mol×K	813.36	Joback Method
cpg	917.02	J/mol×K	843.14	Joback Method
cpg	931.16	J/mol×K	872.92	Joback Method
cpg	944.52	J/mol×K	902.70	Joback Method
cpg	957.15	J/mol×K	932.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358078&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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