2-Fluoro-6-trifluoromethylbenzamide, N,N-dihexyl-

Inchi: InChI=1S/C20H29F4NO/c1-3-5-7-9-14-25(15-10-8-6-4-2)19(26)18-16(20(22,23)24)12-11

InchiKey: BVNWQTREYKISIQ-UHFFFAOYSA-N

Formula: C20H29F4NO

SMILES: CCCCCCN(CCCCCC)C(=O)c1c(F)cccc1C(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	2153.00		NIST Webbook
rinpol	2153.00		NIST Webbook
tb	753.80	K	Joback Method
tc	932.48	K	Joback Method
tf	453.80	K	Joback Method
vc	1.133	m3/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

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=U358115&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