3-Fluoro-5-trifluoromethylbenzamide, N,N-di(2-ethylhexyl)-

Inchi: InChI=1S/C24H37F4NO/c1-5-9-11-18(7-3)16-29(17-19(8-4)12-10-6-2)23(30)20-13-21(24

InchiKey: QOBCNXAARRCMRP-UHFFFAOYSA-N

Formula: C24H37F4NO

SMILES: CCCCC(CC)CN(CC(CC)CCCC)C(=O)c1cc(F)cc(C(F)(F)F)c1

Mol. weight [g/mol]: 431.55

Physical Properties

Property code	Value	Unit	Source
gf	-555.07	kJ/mol	Joback Method
hf	-1173.90	kJ/mol	Joback Method
hfus	53.66	kJ/mol	Joback Method
hvap	76.07	kJ/mol	Joback Method
log10ws	-8.43		Crippen Method
logp	7.720		Crippen Method
mcvol	343.890	ml/mol	McGowan Method
pc	915.50	kPa	Joback Method
rinpol	2171.00		NIST Webbook
rinpol	2171.00		NIST Webbook
tb	844.44	K	Joback Method
tc	1035.03	K	Joback Method
tf	468.88	K	Joback Method
vc	1.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1109.87	J/mol×K	844.44	Joback Method
cpg	1128.38	J/mol×K	876.21	Joback Method
cpg	1145.80	J/mol×K	907.97	Joback Method
cpg	1162.20	J/mol×K	939.74	Joback Method
cpg	1177.66	J/mol×K	971.50	Joback Method
cpg	1192.24	J/mol×K	1003.27	Joback Method
cpg	1206.02	J/mol×K	1035.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358149&Units=SI
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

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