Benzamide, 2,4,5-trifluoro-3-methoxy-N-undecyl-

Inchi: InChI=1S/C19H28F3NO2/c1-3-4-5-6-7-8-9-10-11-12-23-19(24)14-13-15(20)17(22)18(25-

InchiKey: NVAXVQXDSJNFMX-UHFFFAOYSA-N

Formula: C19H28F3NO2

SMILES: CCCCCCCCCCCNC(=O)c1cc(F)c(F)c(OC)c1F

Mol. weight [g/mol]: 359.43

Physical Properties

Property code	Value	Unit	Source
gf	-545.97	kJ/mol	Joback Method
hf	-1024.50	kJ/mol	Joback Method
hfus	54.58	kJ/mol	Joback Method
hvap	75.95	kJ/mol	Joback Method
log10ws	-7.12		Crippen Method
logp	5.373		Crippen Method
mcvol	277.540	ml/mol	McGowan Method
pc	1233.74	kPa	Joback Method
rinpol	2444.00		NIST Webbook
rinpol	2444.00		NIST Webbook
tb	804.99	K	Joback Method
tc	991.14	K	Joback Method
tf	506.98	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.50	J/mol×K	804.99	Joback Method
cpg	866.23	J/mol×K	836.02	Joback Method
cpg	881.04	J/mol×K	867.04	Joback Method
cpg	894.94	J/mol×K	898.07	Joback Method
cpg	907.96	J/mol×K	929.09	Joback Method
cpg	920.11	J/mol×K	960.12	Joback Method
cpg	931.42	J/mol×K	991.14	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=U407648&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