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

Inchi: InChI=1S/C11H12F3NO2/c1-3-4-15-11(16)6-5-7(12)9(14)10(17-2)8(6)13/h5H,3-4H2,1-2H

InchiKey: BHIPCTDZLLCEPL-UHFFFAOYSA-N

Formula: C11H12F3NO2

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

Mol. weight [g/mol]: 247.21

Physical Properties

Property code	Value	Unit	Source
gf	-613.33	kJ/mol	Joback Method
hf	-859.38	kJ/mol	Joback Method
hfus	33.86	kJ/mol	Joback Method
hvap	58.14	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	2.252		Crippen Method
mcvol	164.820	ml/mol	McGowan Method
pc	2313.61	kPa	Joback Method
rinpol	1624.00		NIST Webbook
rinpol	1624.00		NIST Webbook
tb	621.95	K	Joback Method
tc	809.03	K	Joback Method
tf	416.82	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.93	J/mol×K	621.95	Joback Method
cpg	429.58	J/mol×K	653.13	Joback Method
cpg	440.67	J/mol×K	684.31	Joback Method
cpg	451.20	J/mol×K	715.49	Joback Method
cpg	461.17	J/mol×K	746.67	Joback Method
cpg	470.59	J/mol×K	777.85	Joback Method
cpg	479.45	J/mol×K	809.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407636&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

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