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

Inchi: InChI=1S/C12H14F3NO2/c1-3-4-5-16-12(17)7-6-8(13)10(15)11(18-2)9(7)14/h6H,3-5H2,1
InchiKey: XQTBTPRQVOQMRP-UHFFFAOYSA-N
Formula: C12H14F3NO2
SMILES: CCCCNC(=O)c1cc(F)c(F)c(OC)c1F
Mol. weight [g/mol]: 261.24

Physical Properties

Property code	Value	Unit	Source
gf	-604.91	kJ/mol	Joback Method
hf	-880.02	kJ/mol	Joback Method
hfus	36.45	kJ/mol	Joback Method
hvap	60.37	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	2.642		Crippen Method
mcvol	178.910	ml/mol	McGowan Method
pc	2113.89	kPa	Joback Method
rinpol	1726.00		NIST Webbook
rinpol	1726.00		NIST Webbook
tb	644.83	K	Joback Method
tc	830.23	K	Joback Method
tf	428.09	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.45	J/mol×K	644.83	Joback Method
cpg	479.79	J/mol×K	675.73	Joback Method
cpg	491.52	J/mol×K	706.63	Joback Method
cpg	502.64	J/mol×K	737.53	Joback Method
cpg	513.17	J/mol×K	768.43	Joback Method
cpg	523.10	J/mol×K	799.33	Joback Method
cpg	532.44	J/mol×K	830.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407638&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