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

Inchi: InChI=1S/C12H14F3NO2/c1-6(2)5-16-12(17)7-4-8(13)10(15)11(18-3)9(7)14/h4,6H,5H2,1

InchiKey: UTSQWYHEOCPZQG-UHFFFAOYSA-N

Formula: C12H14F3NO2

SMILES: COc1c(F)c(F)cc(C(=O)NCC(C)C)c1F

Mol. weight [g/mol]: 261.24

Physical Properties

Property code	Value	Unit	Source
gf	-607.35	kJ/mol	Joback Method
hf	-885.30	kJ/mol	Joback Method
hfus	32.92	kJ/mol	Joback Method
hvap	59.98	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	2.498		Crippen Method
mcvol	178.910	ml/mol	McGowan Method
pc	2129.52	kPa	Joback Method
rinpol	1673.00		NIST Webbook
rinpol	1673.00		NIST Webbook
tb	644.39	K	Joback Method
tc	832.86	K	Joback Method
tf	413.09	K	Joback Method
vc	0.707	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.95	J/mol×K	644.39	Joback Method
cpg	480.52	J/mol×K	675.80	Joback Method
cpg	492.46	J/mol×K	707.21	Joback Method
cpg	503.77	J/mol×K	738.62	Joback Method
cpg	514.45	J/mol×K	770.04	Joback Method
cpg	524.51	J/mol×K	801.45	Joback Method
cpg	533.94	J/mol×K	832.86	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=U407637&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