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

Inchi: InChI=1S/C10H10F3NO2/c1-3-14-10(15)5-4-6(11)8(13)9(16-2)7(5)12/h4H,3H2,1-2H3,(H
InchiKey: RASPRTCNTXKOPA-UHFFFAOYSA-N
Formula: C10H10F3NO2
SMILES: CCNC(=O)c1cc(F)c(F)c(OC)c1F
Mol. weight [g/mol]: 233.19

Physical Properties

Property code	Value	Unit	Source
gf	-621.75	kJ/mol	Joback Method
hf	-838.74	kJ/mol	Joback Method
hfus	31.27	kJ/mol	Joback Method
hvap	55.92	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	1.862		Crippen Method
mcvol	150.730	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
rinpol	1534.00		NIST Webbook
rinpol	1534.00		NIST Webbook
tb	599.07	K	Joback Method
tc	788.13	K	Joback Method
tf	405.55	K	Joback Method
vc	0.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.99	J/mol×K	599.07	Joback Method
cpg	380.86	J/mol×K	630.58	Joback Method
cpg	391.23	J/mol×K	662.09	Joback Method
cpg	401.08	J/mol×K	693.60	Joback Method
cpg	410.42	J/mol×K	725.11	Joback Method
cpg	419.25	J/mol×K	756.62	Joback Method
cpg	427.57	J/mol×K	788.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407635&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