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

Inchi: InChI=1S/C20H30F3NO2/c1-3-4-5-6-7-8-9-10-11-12-13-24-20(25)15-14-16(21)18(23)19(

InchiKey: CYKHGRSWXOJSBI-UHFFFAOYSA-N

Formula: C20H30F3NO2

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

Mol. weight [g/mol]: 373.45

Physical Properties

Property code	Value	Unit	Source
gf	-537.55	kJ/mol	Joback Method
hf	-1045.14	kJ/mol	Joback Method
hfus	57.17	kJ/mol	Joback Method
hvap	78.18	kJ/mol	Joback Method
log10ws	-7.54		Crippen Method
logp	5.763		Crippen Method
mcvol	291.630	ml/mol	McGowan Method
pc	1154.57	kPa	Joback Method
rinpol	2547.00		NIST Webbook
rinpol	2547.00		NIST Webbook
tb	827.87	K	Joback Method
tc	1016.55	K	Joback Method
tf	518.25	K	Joback Method
vc	1.161	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.40	J/mol×K	827.87	Joback Method
cpg	925.54	J/mol×K	859.32	Joback Method
cpg	940.71	J/mol×K	890.76	Joback Method
cpg	954.92	J/mol×K	922.21	Joback Method
cpg	968.19	J/mol×K	953.65	Joback Method
cpg	980.54	J/mol×K	985.10	Joback Method
cpg	992.00	J/mol×K	1016.55	Joback Method

Sources

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=U407649&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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