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

Inchi: InChI=1S/C15H20F3NO2/c1-3-4-5-6-7-8-19-15(20)10-9-11(16)13(18)14(21-2)12(10)17/h

InchiKey: GFDOCSFZTCLEFI-UHFFFAOYSA-N

Formula: C15H20F3NO2

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

Mol. weight [g/mol]: 303.32

Physical Properties

Property code	Value	Unit	Source
gf	-579.65	kJ/mol	Joback Method
hf	-941.94	kJ/mol	Joback Method
hfus	44.22	kJ/mol	Joback Method
hvap	67.05	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	3.813		Crippen Method
mcvol	221.180	ml/mol	McGowan Method
pc	1648.43	kPa	Joback Method
rinpol	2030.00		NIST Webbook
rinpol	2030.00		NIST Webbook
tb	713.47	K	Joback Method
tc	896.11	K	Joback Method
tf	461.90	K	Joback Method
vc	0.880	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.53	J/mol×K	713.47	Joback Method
cpg	638.53	J/mol×K	743.91	Joback Method
cpg	651.80	J/mol×K	774.35	Joback Method
cpg	664.34	J/mol×K	804.79	Joback Method
cpg	676.16	J/mol×K	835.23	Joback Method
cpg	687.27	J/mol×K	865.67	Joback Method
cpg	697.69	J/mol×K	896.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407644&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