Benzamide, 2,4,5-trifluoro-3-methoxy-N-(hept-2-yl)-

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

InchiKey: XDQOHCRZDRCKEG-UHFFFAOYSA-N

Formula: C15H20F3NO2

SMILES: CCCCCC(C)NC(=O)c1cc(F)c(F)c(OC)c1F

Mol. weight [g/mol]: 303.32

Physical Properties

Property code	Value	Unit	Source
gf	-582.09	kJ/mol	Joback Method
hf	-947.22	kJ/mol	Joback Method
hfus	40.69	kJ/mol	Joback Method
hvap	66.66	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	3.811		Crippen Method
mcvol	221.180	ml/mol	McGowan Method
pc	1659.19	kPa	Joback Method
rinpol	1905.00		NIST Webbook
rinpol	1905.00		NIST Webbook
tb	713.03	K	Joback Method
tc	897.98	K	Joback Method
tf	446.90	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.06	J/mol×K	713.03	Joback Method
cpg	639.25	J/mol×K	743.86	Joback Method
cpg	652.69	J/mol×K	774.68	Joback Method
cpg	665.37	J/mol×K	805.51	Joback Method
cpg	677.31	J/mol×K	836.33	Joback Method
cpg	688.52	J/mol×K	867.16	Joback Method
cpg	699.00	J/mol×K	897.98	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=U407641&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