Benzamide, N-tetrahydrofurfuryl-2,3,4-trifluoro-

Inchi: InChI=1S/C12H12F3NO2/c13-9-4-3-8(10(14)11(9)15)12(17)16-6-7-2-1-5-18-7/h3-4,7H,1

InchiKey: IDBKYQDSGBWNNT-UHFFFAOYSA-N

Formula: C12H12F3NO2

SMILES: O=C(NCC1CCCO1)c1ccc(F)c(F)c1F

Mol. weight [g/mol]: 259.22

Physical Properties

Property code	Value	Unit	Source
gf	-539.85	kJ/mol	Joback Method
hf	-807.85	kJ/mol	Joback Method
hfus	37.56	kJ/mol	Joback Method
hvap	62.07	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	2.013		Crippen Method
mcvol	168.050	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
rinpol	1716.00		NIST Webbook
tb	659.66	K	Joback Method
tc	867.35	K	Joback Method
tf	430.81	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.16	J/mol×K	659.66	Joback Method
cpg	474.90	J/mol×K	694.28	Joback Method
cpg	487.75	J/mol×K	728.89	Joback Method
cpg	499.71	J/mol×K	763.51	Joback Method
cpg	510.84	J/mol×K	798.12	Joback Method
cpg	521.16	J/mol×K	832.74	Joback Method
cpg	530.71	J/mol×K	867.35	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=U307173&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