Benzamide, N-tetrahydrofurfuryl-4-trifluoromethyl-

Inchi: InChI=1S/C13H14F3NO2/c14-13(15,16)10-5-3-9(4-6-10)12(18)17-8-11-2-1-7-19-11/h3-6

InchiKey: XACSBSLCRWPCHJ-UHFFFAOYSA-N

Formula: C13H14F3NO2

SMILES: O=C(NCC1CCCO1)c1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 273.25

Physical Properties

Property code	Value	Unit	Source
gf	-509.33	kJ/mol	Joback Method
hf	-814.30	kJ/mol	Joback Method
hfus	33.52	kJ/mol	Joback Method
hvap	61.67	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	2.614		Crippen Method
mcvol	182.140	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method
rinpol	1786.00		NIST Webbook
rinpol	1786.00		NIST Webbook
tb	669.35	K	Joback Method
tc	883.16	K	Joback Method
tf	419.46	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.21	J/mol×K	669.35	Joback Method
cpg	532.30	J/mol×K	704.99	Joback Method
cpg	546.23	J/mol×K	740.62	Joback Method
cpg	559.10	J/mol×K	776.26	Joback Method
cpg	570.96	J/mol×K	811.89	Joback Method
cpg	581.89	J/mol×K	847.53	Joback Method
cpg	591.96	J/mol×K	883.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307245&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