Benzamide, N-tetrahydrofurfuryl-2-chloro-

Inchi: InChI=1S/C12H14ClNO2/c13-11-6-2-1-5-10(11)12(15)14-8-9-4-3-7-16-9/h1-2,5-6,9H,3-4
InchiKey: HOJRGAVTPWHWKA-UHFFFAOYSA-N
Formula: C12H14ClNO2
SMILES: O=C(NCC1CCCO1)c1ccccc1Cl
Mol. weight [g/mol]: 239.70

Physical Properties

Property code	Value	Unit	Source
gf	51.91	kJ/mol	Joback Method
hf	-212.32	kJ/mol	Joback Method
hfus	33.30	kJ/mol	Joback Method
hvap	67.58	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.249		Crippen Method
mcvol	174.980	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
rinpol	1973.00		NIST Webbook
rinpol	1973.00		NIST Webbook
tb	689.32	K	Joback Method
tc	928.11	K	Joback Method
tf	433.92	K	Joback Method
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.06	J/mol×K	689.32	Joback Method
cpg	480.07	J/mol×K	729.12	Joback Method
cpg	493.89	J/mol×K	768.92	Joback Method
cpg	506.57	J/mol×K	808.72	Joback Method
cpg	518.19	J/mol×K	848.51	Joback Method
cpg	528.82	J/mol×K	888.31	Joback Method
cpg	538.51	J/mol×K	928.11	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306977&Units=SI

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