Benzamide, 2-chloro-N-hexyl-

Inchi: InChI=1S/C13H18ClNO/c1-2-3-4-7-10-15-13(16)11-8-5-6-9-12(11)14/h5-6,8-9H,2-4,7,10
InchiKey: GZKUZAGDBBWXSH-UHFFFAOYSA-N
Formula: C13H18ClNO
SMILES: CCCCCCNC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 239.74

Physical Properties

Property code	Value	Unit	Source
gf	109.90	kJ/mol	Joback Method
hf	-161.44	kJ/mol	Joback Method
hfus	33.97	kJ/mol	Joback Method
hvap	65.04	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.650		Crippen Method
mcvol	194.060	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	1986.00		NIST Webbook
rinpol	1986.00		NIST Webbook
tb	669.97	K	Joback Method
tc	879.44	K	Joback Method
tf	407.72	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.84	J/mol×K	669.97	Joback Method
cpg	512.33	J/mol×K	704.88	Joback Method
cpg	525.92	J/mol×K	739.79	Joback Method
cpg	538.64	J/mol×K	774.70	Joback Method
cpg	550.54	J/mol×K	809.62	Joback Method
cpg	561.65	J/mol×K	844.53	Joback Method
cpg	572.02	J/mol×K	879.44	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=U407434&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