Benzamide, 4-chloro-N-ethyl-N-octyl-

Inchi: InChI=1S/C17H26ClNO/c1-3-5-6-7-8-9-14-19(4-2)17(20)15-10-12-16(18)13-11-15/h10-1
InchiKey: ZKRCJPYLGITCOL-UHFFFAOYSA-N
Formula: C17H26ClNO
SMILES: CCCCCCCCN(CC)C(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 295.85

Physical Properties

Property code	Value	Unit	Source
gf	164.97	kJ/mol	Joback Method
hf	-229.94	kJ/mol	Joback Method
hfus	42.25	kJ/mol	Joback Method
hvap	69.55	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.163		Crippen Method
mcvol	250.420	ml/mol	McGowan Method
pc	1587.28	kPa	Joback Method
rinpol	2453.00		NIST Webbook
rinpol	2453.00		NIST Webbook
tb	723.76	K	Joback Method
tc	921.14	K	Joback Method
tf	432.61	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.97	J/mol×K	723.76	Joback Method
cpg	713.74	J/mol×K	756.66	Joback Method
cpg	729.52	J/mol×K	789.55	Joback Method
cpg	744.34	J/mol×K	822.45	Joback Method
cpg	758.27	J/mol×K	855.34	Joback Method
cpg	771.36	J/mol×K	888.24	Joback Method
cpg	783.64	J/mol×K	921.14	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=U415330&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