Benzamide, N-(3-chlorophenyl)-4-ethyl-

Inchi: InChI=1S/C15H14ClNO/c1-2-11-6-8-12(9-7-11)15(18)17-14-5-3-4-13(16)10-14/h3-10H,2
InchiKey: QUCAEGXNFCWNHP-UHFFFAOYSA-N
Formula: C15H14ClNO
SMILES: CCc1ccc(C(=O)Nc2cccc(Cl)c2)cc1
Mol. weight [g/mol]: 259.73

Physical Properties

Property code	Value	Unit	Source
gf	229.52	kJ/mol	Joback Method
hf	22.34	kJ/mol	Joback Method
hfus	32.80	kJ/mol	Joback Method
hvap	72.43	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.155		Crippen Method
mcvol	198.480	ml/mol	McGowan Method
pc	2532.82	kPa	Joback Method
rinpol	2384.00		NIST Webbook
rinpol	2384.00		NIST Webbook
tb	747.39	K	Joback Method
tc	989.98	K	Joback Method
tf	469.20	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.34	J/mol×K	747.39	Joback Method
cpg	529.08	J/mol×K	787.82	Joback Method
cpg	541.70	J/mol×K	828.25	Joback Method
cpg	553.24	J/mol×K	868.69	Joback Method
cpg	563.79	J/mol×K	909.12	Joback Method
cpg	573.42	J/mol×K	949.55	Joback Method
cpg	582.19	J/mol×K	989.98	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=U307015&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