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

Inchi: InChI=1S/C17H18ClNO/c1-2-3-5-13-8-10-14(11-9-13)17(20)19-16-7-4-6-15(18)12-16/h4
InchiKey: HFAWWPRHBUTMKX-UHFFFAOYSA-N
Formula: C17H18ClNO
SMILES: CCCCc1ccc(C(=O)Nc2cccc(Cl)c2)cc1
Mol. weight [g/mol]: 287.78

Physical Properties

Property code	Value	Unit	Source
gf	246.36	kJ/mol	Joback Method
hf	-18.94	kJ/mol	Joback Method
hfus	37.98	kJ/mol	Joback Method
hvap	76.88	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	4.935		Crippen Method
mcvol	226.660	ml/mol	McGowan Method
pc	2106.13	kPa	Joback Method
rinpol	2611.00		NIST Webbook
rinpol	2611.00		NIST Webbook
tb	793.15	K	Joback Method
tc	1026.96	K	Joback Method
tf	491.74	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.12	J/mol×K	793.15	Joback Method
cpg	637.51	J/mol×K	832.12	Joback Method
cpg	650.76	J/mol×K	871.09	Joback Method
cpg	662.95	J/mol×K	910.06	Joback Method
cpg	674.15	J/mol×K	949.02	Joback Method
cpg	684.43	J/mol×K	987.99	Joback Method
cpg	693.86	J/mol×K	1026.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306992&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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