Benzamide, 3-chloro-N-(3-chlorobenzoyl)-N-propyl-

Inchi: InChI=1S/C17H15Cl2NO2/c1-2-9-20(16(21)12-5-3-7-14(18)10-12)17(22)13-6-4-8-15(19)
InchiKey: IDZAMFRZIBZIIC-UHFFFAOYSA-N
Formula: C17H15Cl2NO2
SMILES: CCCN(C(=O)c1cccc(Cl)c1)C(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 336.21

Physical Properties

Property code	Value	Unit	Source
gf	126.90	kJ/mol	Joback Method
hf	-133.20	kJ/mol	Joback Method
hfus	41.70	kJ/mol	Joback Method
hvap	83.62	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	4.686		Crippen Method
mcvol	240.470	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	2344.00		NIST Webbook
rinpol	2344.00		NIST Webbook
tb	846.72	K	Joback Method
tc	1086.64	K	Joback Method
tf	551.40	K	Joback Method
vc	0.899	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.01	J/mol×K	846.72	Joback Method
cpg	657.10	J/mol×K	886.71	Joback Method
cpg	668.13	J/mol×K	926.69	Joback Method
cpg	678.17	J/mol×K	966.68	Joback Method
cpg	687.32	J/mol×K	1006.67	Joback Method
cpg	695.66	J/mol×K	1046.65	Joback Method
cpg	703.29	J/mol×K	1086.64	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=U407990&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