Benzamide, 3-chloro-N-(3-chlorobenzoyl)-N-(2-ethylhexyl)-

Inchi: InChI=1S/C22H25Cl2NO2/c1-3-5-8-16(4-2)15-25(21(26)17-9-6-11-19(23)13-17)22(27)18
InchiKey: KGOPMVDXRGETIU-UHFFFAOYSA-N
Formula: C22H25Cl2NO2
SMILES: CCCCC(CC)CN(C(=O)c1cccc(Cl)c1)C(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 406.35

Physical Properties

Property code	Value	Unit	Source
gf	166.56	kJ/mol	Joback Method
hf	-241.68	kJ/mol	Joback Method
hfus	51.13	kJ/mol	Joback Method
hvap	94.36	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	6.492		Crippen Method
mcvol	310.920	ml/mol	McGowan Method
pc	1434.80	kPa	Joback Method
rinpol	2714.00		NIST Webbook
rinpol	2714.00		NIST Webbook
tb	960.68	K	Joback Method
tc	1192.77	K	Joback Method
tf	592.75	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	930.83	J/mol×K	960.68	Joback Method
cpg	944.13	J/mol×K	999.36	Joback Method
cpg	956.37	J/mol×K	1038.04	Joback Method
cpg	967.65	J/mol×K	1076.72	Joback Method
cpg	978.06	J/mol×K	1115.40	Joback Method
cpg	987.71	J/mol×K	1154.09	Joback Method
cpg	996.70	J/mol×K	1192.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407994&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

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