Benzamide, 2-chloro-N-(2-chlorobenzoyl)-N-ethyl-

Inchi: InChI=1S/C16H13Cl2NO2/c1-2-19(15(20)11-7-3-5-9-13(11)17)16(21)12-8-4-6-10-14(12)
InchiKey: YXHJMGZYDMYUBU-UHFFFAOYSA-N
Formula: C16H13Cl2NO2
SMILES: CCN(C(=O)c1ccccc1Cl)C(=O)c1ccccc1Cl
Mol. weight [g/mol]: 322.19

Physical Properties

Property code	Value	Unit	Source
gf	118.48	kJ/mol	Joback Method
hf	-112.56	kJ/mol	Joback Method
hfus	39.11	kJ/mol	Joback Method
hvap	81.39	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.296		Crippen Method
mcvol	226.380	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
rinpol	2341.00		NIST Webbook
rinpol	2341.00		NIST Webbook
tb	823.84	K	Joback Method
tc	1067.81	K	Joback Method
tf	540.13	K	Joback Method
vc	0.844	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.49	J/mol×K	823.84	Joback Method
cpg	602.28	J/mol×K	864.50	Joback Method
cpg	612.98	J/mol×K	905.16	Joback Method
cpg	622.70	J/mol×K	945.83	Joback Method
cpg	631.52	J/mol×K	986.49	Joback Method
cpg	639.52	J/mol×K	1027.15	Joback Method
cpg	646.79	J/mol×K	1067.81	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=U407494&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