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

Inchi: InChI=1S/C22H25Cl2NO2/c1-2-3-4-5-6-11-16-25(21(26)17-12-7-9-14-19(17)23)22(27)18
InchiKey: RXBIQKQFQROWJQ-UHFFFAOYSA-N
Formula: C22H25Cl2NO2
SMILES: CCCCCCCCN(C(=O)c1ccccc1Cl)C(=O)c1ccccc1Cl
Mol. weight [g/mol]: 406.35

Physical Properties

Property code	Value	Unit	Source
gf	169.00	kJ/mol	Joback Method
hf	-236.40	kJ/mol	Joback Method
hfus	54.65	kJ/mol	Joback Method
hvap	94.75	kJ/mol	Joback Method
log10ws	-7.88		Crippen Method
logp	6.637		Crippen Method
mcvol	310.920	ml/mol	McGowan Method
pc	1426.15	kPa	Joback Method
rinpol	2930.00		NIST Webbook
rinpol	2930.00		NIST Webbook
tb	961.12	K	Joback Method
tc	1191.09	K	Joback Method
tf	607.75	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	930.38	J/mol×K	961.12	Joback Method
cpg	943.62	J/mol×K	999.45	Joback Method
cpg	955.84	J/mol×K	1037.78	Joback Method
cpg	967.12	J/mol×K	1076.10	Joback Method
cpg	977.56	J/mol×K	1114.43	Joback Method
cpg	987.27	J/mol×K	1152.76	Joback Method
cpg	996.34	J/mol×K	1191.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407502&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