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

Inchi: InChI=1S/C21H23Cl2NO2/c1-2-3-4-5-10-15-24(20(25)16-11-6-8-13-18(16)22)21(26)17-1
InchiKey: QPODEHDCYMWERY-UHFFFAOYSA-N
Formula: C21H23Cl2NO2
SMILES: CCCCCCCN(C(=O)c1ccccc1Cl)C(=O)c1ccccc1Cl
Mol. weight [g/mol]: 392.32

Physical Properties

Property code	Value	Unit	Source
gf	160.58	kJ/mol	Joback Method
hf	-215.76	kJ/mol	Joback Method
hfus	52.06	kJ/mol	Joback Method
hvap	92.52	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	6.246		Crippen Method
mcvol	296.830	ml/mol	McGowan Method
pc	1535.46	kPa	Joback Method
rinpol	2824.00		NIST Webbook
rinpol	2824.00		NIST Webbook
tb	938.24	K	Joback Method
tc	1168.69	K	Joback Method
tf	596.48	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.78	J/mol×K	938.24	Joback Method
cpg	884.81	J/mol×K	976.65	Joback Method
cpg	896.80	J/mol×K	1015.06	Joback Method
cpg	907.85	J/mol×K	1053.47	Joback Method
cpg	918.06	J/mol×K	1091.88	Joback Method
cpg	927.51	J/mol×K	1130.28	Joback Method
cpg	936.30	J/mol×K	1168.69	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=U407501&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