3-Chlorobenzoic acid, N,N-dihexyl-

Inchi: InChI=1S/C19H30ClNO/c1-3-5-7-9-14-21(15-10-8-6-4-2)19(22)17-12-11-13-18(20)16-17
InchiKey: BCRUNUYUUYNQKX-UHFFFAOYSA-N
Formula: C19H30ClNO
SMILES: CCCCCCN(CCCCCC)C(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 323.90

Physical Properties

Property code	Value	Unit	Source
gf	181.81	kJ/mol	Joback Method
hf	-271.22	kJ/mol	Joback Method
hfus	47.43	kJ/mol	Joback Method
hvap	74.00	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	5.943		Crippen Method
mcvol	278.600	ml/mol	McGowan Method
pc	1369.71	kPa	Joback Method
rinpol	2355.00		NIST Webbook
rinpol	2355.00		NIST Webbook
tb	769.52	K	Joback Method
tc	964.77	K	Joback Method
tf	455.15	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	810.83	J/mol×K	769.52	Joback Method
cpg	828.12	J/mol×K	802.06	Joback Method
cpg	844.40	J/mol×K	834.60	Joback Method
cpg	859.71	J/mol×K	867.14	Joback Method
cpg	874.10	J/mol×K	899.68	Joback Method
cpg	887.64	J/mol×K	932.22	Joback Method
cpg	900.37	J/mol×K	964.77	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=U360145&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