3-Chloro-2-fluorobenzamide, N,N-di(2-ethylhexyl)-

Inchi: InChI=1S/C23H37ClFNO/c1-5-9-12-18(7-3)16-26(17-19(8-4)13-10-6-2)23(27)20-14-11-1
InchiKey: AWAWQDIGVGLVST-UHFFFAOYSA-N
Formula: C23H37ClFNO
SMILES: CCCCC(CC)CN(CC(CC)CCCC)C(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 398.00

Physical Properties

Property code	Value	Unit	Source
gf	6.17	kJ/mol	Joback Method
hf	-571.92	kJ/mol	Joback Method
hfus	53.44	kJ/mol	Joback Method
hvap	81.97	kJ/mol	Joback Method
log10ws	-8.01		Crippen Method
logp	7.354		Crippen Method
mcvol	336.730	ml/mol	McGowan Method
pc	1020.73	kPa	Joback Method
rinpol	2549.00		NIST Webbook
tb	864.41	K	Joback Method
tc	1063.01	K	Joback Method
tf	483.34	K	Joback Method
vc	1.294	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.42	J/mol×K	864.41	Joback Method
cpg	1075.52	J/mol×K	897.51	Joback Method
cpg	1092.51	J/mol×K	930.61	Joback Method
cpg	1108.44	J/mol×K	963.71	Joback Method
cpg	1123.39	J/mol×K	996.81	Joback Method
cpg	1137.41	J/mol×K	1029.91	Joback Method
cpg	1150.56	J/mol×K	1063.01	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=U358137&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