Benzamide, 3-chloro-N-(2-ethylhexyl)-

Inchi: InChI=1S/C15H22ClNO/c1-3-5-7-12(4-2)11-17-15(18)13-8-6-9-14(16)10-13/h6,8-10,12H
InchiKey: LIJLHSKPHYMOAL-UHFFFAOYSA-N
Formula: C15H22ClNO
SMILES: CCCCC(CC)CNC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 267.79

Physical Properties

Property code	Value	Unit	Source
gf	124.30	kJ/mol	Joback Method
hf	-208.00	kJ/mol	Joback Method
hfus	35.63	kJ/mol	Joback Method
hvap	69.10	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.286		Crippen Method
mcvol	222.240	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	2150.00		NIST Webbook
rinpol	2150.00		NIST Webbook
tb	715.29	K	Joback Method
tc	922.73	K	Joback Method
tf	415.26	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.34	J/mol×K	715.29	Joback Method
cpg	619.94	J/mol×K	749.86	Joback Method
cpg	634.56	J/mol×K	784.44	Joback Method
cpg	648.24	J/mol×K	819.01	Joback Method
cpg	661.03	J/mol×K	853.58	Joback Method
cpg	672.98	J/mol×K	888.16	Joback Method
cpg	684.12	J/mol×K	922.73	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=U407980&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