Benzamide, 2-chloro-N-octyl-

Inchi: InChI=1S/C15H22ClNO/c1-2-3-4-5-6-9-12-17-15(18)13-10-7-8-11-14(13)16/h7-8,10-11H
InchiKey: WGRXJVIEUFBCJX-UHFFFAOYSA-N
Formula: C15H22ClNO
SMILES: CCCCCCCCNC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 267.79

Physical Properties

Property code	Value	Unit	Source
gf	126.74	kJ/mol	Joback Method
hf	-202.72	kJ/mol	Joback Method
hfus	39.15	kJ/mol	Joback Method
hvap	69.49	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	4.430		Crippen Method
mcvol	222.240	ml/mol	McGowan Method
pc	1885.44	kPa	Joback Method
rinpol	2201.00		NIST Webbook
rinpol	2201.00		NIST Webbook
tb	715.73	K	Joback Method
tc	919.83	K	Joback Method
tf	430.26	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.81	J/mol×K	715.73	Joback Method
cpg	619.14	J/mol×K	749.75	Joback Method
cpg	633.53	J/mol×K	783.76	Joback Method
cpg	647.02	J/mol×K	817.78	Joback Method
cpg	659.66	J/mol×K	851.79	Joback Method
cpg	671.49	J/mol×K	885.81	Joback Method
cpg	682.55	J/mol×K	919.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407437&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

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