Benzamide, 3-chloro-N-heptyl-

Inchi: InChI=1S/C14H20ClNO/c1-2-3-4-5-6-10-16-14(17)12-8-7-9-13(15)11-12/h7-9,11H,2-6,10
InchiKey: SCYWBGROYTZINS-UHFFFAOYSA-N
Formula: C14H20ClNO
SMILES: CCCCCCCNC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 253.77

Physical Properties

Property code	Value	Unit	Source
gf	118.32	kJ/mol	Joback Method
hf	-182.08	kJ/mol	Joback Method
hfus	36.56	kJ/mol	Joback Method
hvap	67.26	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.040		Crippen Method
mcvol	208.150	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	2160.00		NIST Webbook
rinpol	2160.00		NIST Webbook
tb	692.85	K	Joback Method
tc	899.43	K	Joback Method
tf	418.99	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.20	J/mol×K	692.85	Joback Method
cpg	565.14	J/mol×K	727.28	Joback Method
cpg	579.16	J/mol×K	761.71	Joback Method
cpg	592.29	J/mol×K	796.14	Joback Method
cpg	604.59	J/mol×K	830.57	Joback Method
cpg	616.08	J/mol×K	865.00	Joback Method
cpg	626.82	J/mol×K	899.43	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=U407981&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