Benzamide, 3-chloro-N-(hept-2-yl)-

Inchi: InChI=1S/C14H20ClNO/c1-3-4-5-7-11(2)16-14(17)12-8-6-9-13(15)10-12/h6,8-11H,3-5,7H
InchiKey: KFYLNOODNSMBNA-UHFFFAOYSA-N
Formula: C14H20ClNO
SMILES: CCCCCC(C)NC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 253.77

Physical Properties

Property code	Value	Unit	Source
gf	115.88	kJ/mol	Joback Method
hf	-187.36	kJ/mol	Joback Method
hfus	33.04	kJ/mol	Joback Method
hvap	66.88	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.039		Crippen Method
mcvol	208.150	ml/mol	McGowan Method
pc	2068.00	kPa	Joback Method
rinpol	2016.00		NIST Webbook
rinpol	2016.00		NIST Webbook
tb	692.41	K	Joback Method
tc	902.61	K	Joback Method
tf	403.99	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.72	J/mol×K	692.41	Joback Method
cpg	565.95	J/mol×K	727.44	Joback Method
cpg	580.21	J/mol×K	762.48	Joback Method
cpg	593.55	J/mol×K	797.51	Joback Method
cpg	606.01	J/mol×K	832.54	Joback Method
cpg	617.63	J/mol×K	867.57	Joback Method
cpg	628.46	J/mol×K	902.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407978&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