Benzamide, 4-chloro-N-ethyl-N-hept-2-yl-

Inchi: InChI=1S/C16H24ClNO/c1-4-6-7-8-13(3)18(5-2)16(19)14-9-11-15(17)12-10-14/h9-13H,4
InchiKey: LWHHQIZZEOLVHI-UHFFFAOYSA-N
Formula: C16H24ClNO
SMILES: CCCCCC(C)N(CC)C(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 281.82

Physical Properties

Property code	Value	Unit	Source
gf	154.11	kJ/mol	Joback Method
hf	-214.58	kJ/mol	Joback Method
hfus	36.14	kJ/mol	Joback Method
hvap	66.93	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.771		Crippen Method
mcvol	236.330	ml/mol	McGowan Method
pc	1727.46	kPa	Joback Method
rinpol	2138.00		NIST Webbook
rinpol	2138.00		NIST Webbook
tb	700.44	K	Joback Method
tc	902.86	K	Joback Method
tf	406.34	K	Joback Method
vc	0.890	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	642.15	J/mol×K	700.44	Joback Method
cpg	658.91	J/mol×K	734.18	Joback Method
cpg	674.65	J/mol×K	767.91	Joback Method
cpg	689.41	J/mol×K	801.65	Joback Method
cpg	703.24	J/mol×K	835.39	Joback Method
cpg	716.19	J/mol×K	869.12	Joback Method
cpg	728.32	J/mol×K	902.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415326&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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