Benzamide, 4-chloro-N-ethyl-N-octadecyl-

Inchi: InChI=1S/C27H46ClNO/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-24-29(4-2)27(30)
InchiKey: JSEPPRIKQIHTLD-UHFFFAOYSA-N
Formula: C27H46ClNO
SMILES: CCCCCCCCCCCCCCCCCCN(CC)C(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 436.11

Physical Properties

Property code	Value	Unit	Source
gf	249.17	kJ/mol	Joback Method
hf	-436.34	kJ/mol	Joback Method
hfus	68.16	kJ/mol	Joback Method
hvap	91.81	kJ/mol	Joback Method
log10ws	-9.84		Crippen Method
logp	9.064		Crippen Method
mcvol	391.320	ml/mol	McGowan Method
pc	830.50	kPa	Joback Method
rinpol	1160.00		NIST Webbook
rinpol	1160.00		NIST Webbook
tb	952.56	K	Joback Method
tc	1166.43	K	Joback Method
tf	545.31	K	Joback Method
vc	1.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1299.76	J/mol×K	952.56	Joback Method
cpg	1319.71	J/mol×K	988.21	Joback Method
cpg	1338.42	J/mol×K	1023.85	Joback Method
cpg	1355.97	J/mol×K	1059.50	Joback Method
cpg	1372.46	J/mol×K	1095.14	Joback Method
cpg	1387.99	J/mol×K	1130.79	Joback Method
cpg	1402.64	J/mol×K	1166.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415337&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