

Benzamide, 4-chloro-N-ethyl-N-2-ethylhexyl-

Inchi:	InChI=1S/C17H26ClNO/c1-4-7-8-14(5-2)13-19(6-3)17(20)15-9-11-16(18)12-10-15/h9-12
InchiKey:	NTIXVOUDDPUFFR-UHFFFAOYSA-N
Formula:	C17H26ClNO
SMILES:	CCCCC(CC)CN(CC)C(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	295.85

Physical Properties

Property code	Value	Unit	Source
gf	162.53	kJ/mol	Joback Method
hf	-235.22	kJ/mol	Joback Method
hfus	38.73	kJ/mol	Joback Method
hvap	69.16	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	5.018		Crippen Method
mvol	250.420	ml/mol	McGowan Method
pc	1597.44	kPa	Joback Method
rinpol	2245.00		NIST Webbook
rinpol	2245.00		NIST Webbook
tb	723.32	K	Joback Method
tc	923.67	K	Joback Method
tf	417.61	K	Joback Method
vc	0.947	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	697.48	J/molxK	723.32	Joback Method
cpg	714.52	J/molxK	756.71	Joback Method
cpg	730.52	J/molxK	790.10	Joback Method
cpg	745.54	J/molxK	823.49	Joback Method
cpg	759.63	J/molxK	856.88	Joback Method
cpg	772.84	J/molxK	890.27	Joback Method
cpg	785.21	J/molxK	923.67	Joback Method

Sources

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=U415328&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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