Benzamide, 4-chloro-N-ethyl-N-heptyl-

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

Physical Properties

Property code	Value	Unit	Source
gf	156.55	kJ/mol	Joback Method
hf	-209.30	kJ/mol	Joback Method
hfus	39.66	kJ/mol	Joback Method
hvap	67.32	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	4.772		Crippen Method
mcvol	236.330	ml/mol	McGowan Method
pc	1716.03	kPa	Joback Method
rinpol	2349.00		NIST Webbook
rinpol	2349.00		NIST Webbook
tb	700.88	K	Joback Method
tc	900.06	K	Joback Method
tf	421.34	K	Joback Method
vc	0.896	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.65	J/mol×K	700.88	Joback Method
cpg	658.12	J/mol×K	734.08	Joback Method
cpg	673.61	J/mol×K	767.27	Joback Method
cpg	688.16	J/mol×K	800.47	Joback Method
cpg	701.82	J/mol×K	833.67	Joback Method
cpg	714.63	J/mol×K	866.86	Joback Method
cpg	726.66	J/mol×K	900.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415329&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

Latest version available from:
https://www.chemeo.com/cid/119-516-7/Benzamide-4-chloro-N-ethyl-N-heptyl.pdf
Generated by Cheméo on 2024-04-29 12:22:06.120182255 +0000 UTC m=+16682575.040759570.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.