Benzamide, N,N-diheptyl-4-chloro-

Inchi: InChI=1S/C21H34ClNO/c1-3-5-7-9-11-17-23(18-12-10-8-6-4-2)21(24)19-13-15-20(22)16
InchiKey: WLIIKSWZVDTDSF-UHFFFAOYSA-N
Formula: C21H34ClNO
SMILES: CCCCCCCN(CCCCCCC)C(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 351.95

Physical Properties

Property code	Value	Unit	Source
gf	198.65	kJ/mol	Joback Method
hf	-312.50	kJ/mol	Joback Method
hfus	52.62	kJ/mol	Joback Method
hvap	78.45	kJ/mol	Joback Method
log10ws	-7.32		Crippen Method
logp	6.723		Crippen Method
mcvol	306.780	ml/mol	McGowan Method
pc	1194.00	kPa	Joback Method
rinpol	2475.00		NIST Webbook
rinpol	2475.00		NIST Webbook
tb	815.28	K	Joback Method
tc	1010.68	K	Joback Method
tf	477.69	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	928.52	J/mol×K	815.28	Joback Method
cpg	946.31	J/mol×K	847.85	Joback Method
cpg	963.05	J/mol×K	880.41	Joback Method
cpg	978.81	J/mol×K	912.98	Joback Method
cpg	993.63	J/mol×K	945.55	Joback Method
cpg	1007.58	J/mol×K	978.11	Joback Method
cpg	1020.71	J/mol×K	1010.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308590&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