Benzamide, N-heptyl-N-octyl-4-chloro-

Inchi: InChI=1S/C22H36ClNO/c1-3-5-7-9-11-13-19-24(18-12-10-8-6-4-2)22(25)20-14-16-21(23
InchiKey: YNGWSACUMIXQBU-UHFFFAOYSA-N
Formula: C22H36ClNO
SMILES: CCCCCCCCN(CCCCCCC)C(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 365.98

Physical Properties

Property code	Value	Unit	Source
gf	207.07	kJ/mol	Joback Method
hf	-333.14	kJ/mol	Joback Method
hfus	55.21	kJ/mol	Joback Method
hvap	80.68	kJ/mol	Joback Method
log10ws	-7.74		Crippen Method
logp	7.113		Crippen Method
mcvol	320.870	ml/mol	McGowan Method
pc	1118.56	kPa	Joback Method
rinpol	2574.00		NIST Webbook
rinpol	2574.00		NIST Webbook
tb	838.16	K	Joback Method
tc	1034.62	K	Joback Method
tf	488.96	K	Joback Method
vc	1.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	988.64	J/mol×K	838.16	Joback Method
cpg	1006.70	J/mol×K	870.90	Joback Method
cpg	1023.69	J/mol×K	903.65	Joback Method
cpg	1039.67	J/mol×K	936.39	Joback Method
cpg	1054.71	J/mol×K	969.13	Joback Method
cpg	1068.87	J/mol×K	1001.88	Joback Method
cpg	1082.20	J/mol×K	1034.62	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=U308591&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume