Benzamide, N-ethyl-N-(3-methylphenyl)-4-chloro-

Inchi: InChI=1S/C16H16ClNO/c1-3-18(15-6-4-5-12(2)11-15)16(19)13-7-9-14(17)10-8-13/h4-11
InchiKey: MHIIVAZRXRPBPI-UHFFFAOYSA-N
Formula: C16H16ClNO
SMILES: CCN(C(=O)c1ccc(Cl)cc1)c1cccc(C)c1
Mol. weight [g/mol]: 273.76

Physical Properties

Property code	Value	Unit	Source
gf	259.33	kJ/mol	Joback Method
hf	15.76	kJ/mol	Joback Method
hfus	33.32	kJ/mol	Joback Method
hvap	70.26	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.315		Crippen Method
mcvol	212.570	ml/mol	McGowan Method
pc	2271.90	kPa	Joback Method
rinpol	1985.00		NIST Webbook
tb	732.54	K	Joback Method
tc	969.35	K	Joback Method
tf	460.28	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.86	J/mol×K	732.54	Joback Method
cpg	570.92	J/mol×K	772.01	Joback Method
cpg	584.79	J/mol×K	811.48	Joback Method
cpg	597.53	J/mol×K	850.95	Joback Method
cpg	609.24	J/mol×K	890.42	Joback Method
cpg	619.99	J/mol×K	929.89	Joback Method
cpg	629.86	J/mol×K	969.35	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308587&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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