Benzamide, N-ethyl-N-(3-methylphenyl)-3-methyl-

Inchi: InChI=1S/C17H19NO/c1-4-18(16-10-6-8-14(3)12-16)17(19)15-9-5-7-13(2)11-15/h5-12H,

InchiKey: PVKJASZGPBQRHL-UHFFFAOYSA-N

Formula: C17H19NO

SMILES: CCN(C(=O)c1cccc(C)c1)c1cccc(C)c1

Mol. weight [g/mol]: 253.34

Physical Properties

Property code	Value	Unit	Source
gf	279.68	kJ/mol	Joback Method
hf	10.86	kJ/mol	Joback Method
hfus	31.71	kJ/mol	Joback Method
hvap	68.10	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	3.970		Crippen Method
mcvol	214.420	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
rinpol	1935.00		NIST Webbook
rinpol	1935.00		NIST Webbook
tb	717.99	K	Joback Method
tc	947.89	K	Joback Method
tf	441.63	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.08	J/mol×K	717.99	Joback Method
cpg	599.81	J/mol×K	756.31	Joback Method
cpg	615.30	J/mol×K	794.62	Joback Method
cpg	629.62	J/mol×K	832.94	Joback Method
cpg	642.85	J/mol×K	871.25	Joback Method
cpg	655.07	J/mol×K	909.57	Joback Method
cpg	666.34	J/mol×K	947.89	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308555&Units=SI

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