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

Inchi: InChI=1S/C16H17NO/c1-3-13-7-9-14(10-8-13)16(18)17-15-6-4-5-12(2)11-15/h4-11H,3H2
InchiKey: HUVBOWFSUKATRD-UHFFFAOYSA-N
Formula: C16H17NO
SMILES: CCc1ccc(C(=O)Nc2cccc(C)c2)cc1
Mol. weight [g/mol]: 239.31

Physical Properties

Property code	Value	Unit	Source
gf	249.87	kJ/mol	Joback Method
hf	17.44	kJ/mol	Joback Method
hfus	31.20	kJ/mol	Joback Method
hvap	70.27	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	3.810		Crippen Method
mcvol	200.330	ml/mol	McGowan Method
pc	2388.85	kPa	Joback Method
rinpol	2267.00		NIST Webbook
tb	732.84	K	Joback Method
tc	968.43	K	Joback Method
tf	450.55	K	Joback Method
vc	0.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.83	J/mol×K	732.84	Joback Method
cpg	559.26	J/mol×K	772.10	Joback Method
cpg	573.51	J/mol×K	811.37	Joback Method
cpg	586.64	J/mol×K	850.63	Joback Method
cpg	598.72	J/mol×K	889.90	Joback Method
cpg	609.82	J/mol×K	929.16	Joback Method
cpg	620.00	J/mol×K	968.43	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=U307014&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