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

Inchi: InChI=1S/C20H25NO/c1-4-6-9-17-11-13-18(14-12-17)20(22)21(5-2)19-10-7-8-16(3)15-19

InchiKey: PGZZJWNPIRTSLL-UHFFFAOYSA-N

Formula: C20H25NO

SMILES: CCCCc1ccc(C(=O)N(CC)c2cccc(C)c2)cc1

Mol. weight [g/mol]: 295.42

Physical Properties

Property code	Value	Unit	Source
gf	304.94	kJ/mol	Joback Method
hf	-51.06	kJ/mol	Joback Method
hfus	39.48	kJ/mol	Joback Method
hvap	74.78	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	5.004		Crippen Method
mcvol	256.690	ml/mol	McGowan Method
pc	1672.79	kPa	Joback Method
rinpol	2243.00		NIST Webbook
tb	786.63	K	Joback Method
tc	1006.08	K	Joback Method
tf	475.44	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.02	J/mol×K	786.63	Joback Method
cpg	767.30	J/mol×K	823.21	Joback Method
cpg	783.36	J/mol×K	859.78	Joback Method
cpg	798.29	J/mol×K	896.36	Joback Method
cpg	812.15	J/mol×K	932.93	Joback Method
cpg	825.03	J/mol×K	969.51	Joback Method
cpg	836.99	J/mol×K	1006.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308567&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

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