

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

Inchi:	InChI=1S/C18H21NO/c1-4-15-9-11-16(12-10-15)18(20)19(5-2)17-8-6-7-14(3)13-17/h6-1
InchiKey:	QAZLOYMALKJQLM-UHFFFAOYSA-N
Formula:	C18H21NO
SMILES:	CCc1ccc(C(=O)N(CC)c2cccc(C)c2)cc1
Mol. weight [g/mol]:	267.37

Physical Properties

Property code	Value	Unit	Source
gf	288.10	kJ/mol	Joback Method
hf	-9.78	kJ/mol	Joback Method
hfus	34.30	kJ/mol	Joback Method
hvap	70.33	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.224		Crippen Method
mcvol	228.510	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinsol	2050.00		NIST Webbook
tb	740.87	K	Joback Method
tc	966.79	K	Joback Method
tf	452.90	K	Joback Method
vc	0.852	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.67	J/mol×K	740.87	Joback Method
cpg	654.63	J/mol×K	778.52	Joback Method
cpg	670.35	J/mol×K	816.18	Joback Method
cpg	684.92	J/mol×K	853.83	Joback Method
cpg	698.40	J/mol×K	891.49	Joback Method
cpg	710.88	J/mol×K	929.14	Joback Method
cpg	722.42	J/mol×K	966.79	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=U308544&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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

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