Propanamide, N-ethyl-N-(3-methylphenyl)-3-phenyl-

Inchi: InChI=1S/C18H21NO/c1-3-19(17-11-7-8-15(2)14-17)18(20)13-12-16-9-5-4-6-10-16/h4-1

InchiKey: ZKSPJKQZFHLEIL-UHFFFAOYSA-N

Formula: C18H21NO

SMILES: CCN(C(=O)CCc1ccccc1)c1cccc(C)c1

Mol. weight [g/mol]: 267.37

Physical Properties

Property code	Value	Unit	Source
gf	297.73	kJ/mol	Joback Method
hf	1.69	kJ/mol	Joback Method
hfus	34.69	kJ/mol	Joback Method
hvap	69.67	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.981		Crippen Method
mcvol	228.510	ml/mol	McGowan Method
pc	1996.55	kPa	Joback Method
rinpol	2069.00		NIST Webbook
rinpol	2069.00		NIST Webbook
tb	735.89	K	Joback Method
tc	961.03	K	Joback Method
tf	440.38	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	638.42	J/mol×K	735.89	Joback Method
cpg	655.52	J/mol×K	773.41	Joback Method
cpg	671.36	J/mol×K	810.94	Joback Method
cpg	686.03	J/mol×K	848.46	Joback Method
cpg	699.59	J/mol×K	885.98	Joback Method
cpg	712.14	J/mol×K	923.51	Joback Method
cpg	723.76	J/mol×K	961.03	Joback Method

Sources

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=U308213&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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