Propanamide, N-ethyl-N-(3-methylphenyl)-2,2-dimethyl-

Inchi: InChI=1S/C14H21NO/c1-6-15(13(16)14(3,4)5)12-9-7-8-11(2)10-12/h7-10H,6H2,1-5H3

InchiKey: ZAROPWXBNKPAFL-UHFFFAOYSA-N

Formula: C14H21NO

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

Mol. weight [g/mol]: 219.32

Physical Properties

Property code	Value	Unit	Source
gf	154.48	kJ/mol	Joback Method
hf	-161.03	kJ/mol	Joback Method
hfus	22.87	kJ/mol	Joback Method
hvap	57.19	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.394		Crippen Method
mcvol	195.910	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpol	1522.00		NIST Webbook
tb	614.46	K	Joback Method
tc	826.05	K	Joback Method
tf	371.30	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.66	J/mol×K	614.46	Joback Method
cpg	525.34	J/mol×K	649.73	Joback Method
cpg	541.85	J/mol×K	684.99	Joback Method
cpg	557.26	J/mol×K	720.26	Joback Method
cpg	571.64	J/mol×K	755.52	Joback Method
cpg	585.06	J/mol×K	790.79	Joback Method
cpg	597.58	J/mol×K	826.05	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=U308125&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