Propanamide, N-(3-methylphenyl)-2-methyl-

Inchi: InChI=1S/C11H15NO/c1-8(2)11(13)12-10-6-4-5-9(3)7-10/h4-8H,1-3H3,(H,12,13)
InchiKey: OFKDADAPWXHGJJ-UHFFFAOYSA-N
Formula: C11H15NO
SMILES: Cc1cccc(NC(=O)C(C)C)c1
Mol. weight [g/mol]: 177.24

Physical Properties

Property code	Value	Unit	Source
gf	102.55	kJ/mol	Joback Method
hf	-109.70	kJ/mol	Joback Method
hfus	21.07	kJ/mol	Joback Method
hvap	55.81	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.590		Crippen Method
mcvol	153.640	ml/mol	McGowan Method
pc	2847.48	kPa	Joback Method
rinpol	1542.00		NIST Webbook
tb	586.34	K	Joback Method
tc	803.38	K	Joback Method
tf	340.26	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.15	J/mol×K	586.34	Joback Method
cpg	385.85	J/mol×K	622.51	Joback Method
cpg	399.64	J/mol×K	658.69	Joback Method
cpg	412.56	J/mol×K	694.86	Joback Method
cpg	424.64	J/mol×K	731.03	Joback Method
cpg	435.93	J/mol×K	767.21	Joback Method
cpg	446.44	J/mol×K	803.38	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=U307320&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