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

Inchi: InChI=1S/C12H15NO/c1-9(2)7-12(14)13-11-6-4-5-10(3)8-11/h4-8H,1-3H3,(H,13,14)
InchiKey: BBEWYYXUPWRIRQ-UHFFFAOYSA-N
Formula: C12H15NO
SMILES: CC(C)=CC(=O)Nc1cccc(C)c1
Mol. weight [g/mol]: 189.25

Physical Properties

Property code	Value	Unit	Source
gf	185.08	kJ/mol	Joback Method
hf	-17.63	kJ/mol	Joback Method
hfus	26.08	kJ/mol	Joback Method
hvap	58.46	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.900		Crippen Method
mcvol	163.430	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
rinpol	1733.00		NIST Webbook
tb	613.70	K	Joback Method
tc	835.41	K	Joback Method
tf	347.49	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.67	J/mol×K	613.70	Joback Method
cpg	413.31	J/mol×K	650.65	Joback Method
cpg	426.99	J/mol×K	687.60	Joback Method
cpg	439.76	J/mol×K	724.55	Joback Method
cpg	451.69	J/mol×K	761.51	Joback Method
cpg	462.81	J/mol×K	798.46	Joback Method
cpg	473.20	J/mol×K	835.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307268&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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