Butanamide, N-ethyl-N-(3-methylphenyl)-

Inchi: InChI=1S/C13H19NO/c1-4-7-13(15)14(5-2)12-9-6-8-11(3)10-12/h6,8-10H,4-5,7H2,1-3H3
InchiKey: JNXDPGLADCEVCS-UHFFFAOYSA-N
Formula: C13H19NO
SMILES: CCCC(=O)N(CC)c1cccc(C)c1
Mol. weight [g/mol]: 205.30

Physical Properties

Property code	Value	Unit	Source
gf	143.22	kJ/mol	Joback Method
hf	-131.64	kJ/mol	Joback Method
hfus	27.70	kJ/mol	Joback Method
hvap	56.26	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.148		Crippen Method
mcvol	181.820	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinpol	1516.00		NIST Webbook
rinpol	1516.00		NIST Webbook
tb	594.81	K	Joback Method
tc	797.96	K	Joback Method
tf	357.61	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	453.71	J/mol×K	594.81	Joback Method
cpg	470.05	J/mol×K	628.67	Joback Method
cpg	485.45	J/mol×K	662.53	Joback Method
cpg	499.93	J/mol×K	696.39	Joback Method
cpg	513.54	J/mol×K	730.25	Joback Method
cpg	526.31	J/mol×K	764.10	Joback Method
cpg	538.29	J/mol×K	797.96	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=U308675&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