Hexanamide, N-(3-methylphenyl)-

Inchi: InChI=1S/C13H19NO/c1-3-4-5-9-13(15)14-12-8-6-7-11(2)10-12/h6-8,10H,3-5,9H2,1-2H3
InchiKey: ORZBFCDGVYYOQD-UHFFFAOYSA-N
Formula: C13H19NO
SMILES: CCCCCC(=O)Nc1cccc(C)c1
Mol. weight [g/mol]: 205.30

Physical Properties

Property code	Value	Unit	Source
gf	121.83	kJ/mol	Joback Method
hf	-145.70	kJ/mol	Joback Method
hfus	29.78	kJ/mol	Joback Method
hvap	60.65	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.514		Crippen Method
mcvol	181.820	ml/mol	McGowan Method
pc	2324.78	kPa	Joback Method
rinpol	1804.00		NIST Webbook
tb	632.54	K	Joback Method
tc	838.46	K	Joback Method
tf	377.80	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.96	J/mol×K	632.54	Joback Method
cpg	485.49	J/mol×K	666.86	Joback Method
cpg	500.12	J/mol×K	701.18	Joback Method
cpg	513.87	J/mol×K	735.50	Joback Method
cpg	526.79	J/mol×K	769.82	Joback Method
cpg	538.90	J/mol×K	804.14	Joback Method
cpg	550.24	J/mol×K	838.46	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=U307287&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