Cyclohexanecarboxamide, N-(3-methylphenyl)-

Inchi: InChI=1S/C14H19NO/c1-11-6-5-9-13(10-11)15-14(16)12-7-3-2-4-8-12/h5-6,9-10,12H,2-4

InchiKey: CWVHDXWMBQABJH-UHFFFAOYSA-N

Formula: C14H19NO

SMILES: Cc1cccc(NC(=O)C2CCCCC2)c1

Mol. weight [g/mol]: 217.31

Physical Properties

Property code	Value	Unit	Source
gf	154.70	kJ/mol	Joback Method
hf	-112.02	kJ/mol	Joback Method
hfus	24.20	kJ/mol	Joback Method
hvap	63.31	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.514		Crippen Method
mcvol	185.050	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
rinpol	1966.00		NIST Webbook
rinpol	1966.00		NIST Webbook
tb	674.97	K	Joback Method
tc	912.23	K	Joback Method
tf	396.45	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.97	J/mol×K	674.97	Joback Method
cpg	532.88	J/mol×K	714.51	Joback Method
cpg	550.37	J/mol×K	754.06	Joback Method
cpg	566.49	J/mol×K	793.60	Joback Method
cpg	581.32	J/mol×K	833.14	Joback Method
cpg	594.92	J/mol×K	872.69	Joback Method
cpg	607.34	J/mol×K	912.23	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=U306946&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