Cyclopentanecarboxamide, N-(3-methylphenyl)-

Inchi: InChI=1S/C13H17NO/c1-10-5-4-8-12(9-10)14-13(15)11-6-2-3-7-11/h4-5,8-9,11H,2-3,6-7
InchiKey: UKLIDCZVVSZTGM-UHFFFAOYSA-N
Formula: C13H17NO
SMILES: Cc1cccc(NC(=O)C2CCCC2)c1
Mol. weight [g/mol]: 203.28

Physical Properties

Property code	Value	Unit	Source
gf	158.38	kJ/mol	Joback Method
hf	-85.22	kJ/mol	Joback Method
hfus	23.71	kJ/mol	Joback Method
hvap	60.91	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.124		Crippen Method
mcvol	170.960	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
rinpol	1867.00		NIST Webbook
tb	647.82	K	Joback Method
tc	882.27	K	Joback Method
tf	388.70	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.08	J/mol×K	647.82	Joback Method
cpg	476.80	J/mol×K	686.90	Joback Method
cpg	493.22	J/mol×K	725.97	Joback Method
cpg	508.42	J/mol×K	765.05	Joback Method
cpg	522.45	J/mol×K	804.12	Joback Method
cpg	535.39	J/mol×K	843.20	Joback Method
cpg	547.31	J/mol×K	882.27	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=U307025&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

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