Cyclopropanecarboxamide, N-(3-methylphenyl)-

Inchi: InChI=1S/C11H13NO/c1-8-3-2-4-10(7-8)12-11(13)9-5-6-9/h2-4,7,9H,5-6H2,1H3,(H,12,13

InchiKey: VSELQIUIVXSQKX-UHFFFAOYSA-N

Formula: C11H13NO

SMILES: Cc1cccc(NC(=O)C2CC2)c1

Mol. weight [g/mol]: 175.23

Physical Properties

Property code	Value	Unit	Source
gf	165.74	kJ/mol	Joback Method
hf	-31.62	kJ/mol	Joback Method
hfus	22.73	kJ/mol	Joback Method
hvap	56.11	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.344		Crippen Method
mcvol	142.780	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
rinpol	1675.00		NIST Webbook
rinpol	1675.00		NIST Webbook
tb	593.52	K	Joback Method
tc	821.63	K	Joback Method
tf	373.20	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.04	J/mol×K	593.52	Joback Method
cpg	370.95	J/mol×K	631.54	Joback Method
cpg	384.78	J/mol×K	669.56	Joback Method
cpg	397.62	J/mol×K	707.57	Joback Method
cpg	409.53	J/mol×K	745.59	Joback Method
cpg	420.59	J/mol×K	783.61	Joback Method
cpg	430.88	J/mol×K	821.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307186&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

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