Cyclobutanecarboxamide, N-(3-methylphenyl)-

Inchi: InChI=1S/C12H15NO/c1-9-4-2-7-11(8-9)13-12(14)10-5-3-6-10/h2,4,7-8,10H,3,5-6H2,1H3
InchiKey: FAZSASKSCDHQIE-UHFFFAOYSA-N
Formula: C12H15NO
SMILES: Cc1cccc(NC(=O)C2CCC2)c1
Mol. weight [g/mol]: 189.25

Physical Properties

Property code	Value	Unit	Source
gf	162.06	kJ/mol	Joback Method
hf	-58.42	kJ/mol	Joback Method
hfus	23.22	kJ/mol	Joback Method
hvap	58.51	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	2.734		Crippen Method
mcvol	156.870	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
rinpol	1765.00		NIST Webbook
tb	620.67	K	Joback Method
tc	852.08	K	Joback Method
tf	380.95	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.39	J/mol×K	620.67	Joback Method
cpg	422.76	J/mol×K	659.24	Joback Method
cpg	437.96	J/mol×K	697.81	Joback Method
cpg	452.05	J/mol×K	736.37	Joback Method
cpg	465.11	J/mol×K	774.94	Joback Method
cpg	477.20	J/mol×K	813.51	Joback Method
cpg	488.40	J/mol×K	852.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307047&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