Cyclobutanecarboxamide, N-ethyl-N-(3-methylphenyl)-

Inchi: InChI=1S/C14H19NO/c1-3-15(14(16)12-7-5-8-12)13-9-4-6-11(2)10-13/h4,6,9-10,12H,3,5

InchiKey: MCPWVWKGOLYZBP-UHFFFAOYSA-N

Formula: C14H19NO

SMILES: CCN(C(=O)C1CCC1)c1cccc(C)c1

Mol. weight [g/mol]: 217.31

Physical Properties

Property code	Value	Unit	Source
gf	200.29	kJ/mol	Joback Method
hf	-85.64	kJ/mol	Joback Method
hfus	26.32	kJ/mol	Joback Method
hvap	58.57	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.148		Crippen Method
mcvol	185.050	ml/mol	McGowan Method
pc	2426.65	kPa	Joback Method
rinpol	1650.00		NIST Webbook
rinpol	1650.00		NIST Webbook
tb	628.70	K	Joback Method
tc	849.44	K	Joback Method
tf	383.30	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.35	J/mol×K	628.70	Joback Method
cpg	510.62	J/mol×K	665.49	Joback Method
cpg	527.64	J/mol×K	702.28	Joback Method
cpg	543.47	J/mol×K	739.07	Joback Method
cpg	558.21	J/mol×K	775.86	Joback Method
cpg	571.92	J/mol×K	812.65	Joback Method
cpg	584.68	J/mol×K	849.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308597&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