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

Inchi: InChI=1S/C15H21NO/c1-3-16(14-10-6-7-12(2)11-14)15(17)13-8-4-5-9-13/h6-7,10-11,13H

InchiKey: CYLOTQUVWKVQAD-UHFFFAOYSA-N

Formula: C15H21NO

SMILES: CCN(C(=O)C1CCCC1)c1cccc(C)c1

Mol. weight [g/mol]: 231.33

Physical Properties

Property code	Value	Unit	Source
gf	196.61	kJ/mol	Joback Method
hf	-112.44	kJ/mol	Joback Method
hfus	26.81	kJ/mol	Joback Method
hvap	60.97	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.538		Crippen Method
mcvol	199.140	ml/mol	McGowan Method
pc	2265.42	kPa	Joback Method
rinpol	1716.00		NIST Webbook
rinpol	1716.00		NIST Webbook
tb	655.85	K	Joback Method
tc	879.66	K	Joback Method
tf	391.05	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.42	J/mol×K	655.85	Joback Method
cpg	566.85	J/mol×K	693.15	Joback Method
cpg	584.93	J/mol×K	730.45	Joback Method
cpg	601.73	J/mol×K	767.76	Joback Method
cpg	617.31	J/mol×K	805.06	Joback Method
cpg	631.77	J/mol×K	842.36	Joback Method
cpg	645.15	J/mol×K	879.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308609&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