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

Inchi: InChI=1S/C13H17NO/c1-3-14(13(15)11-7-8-11)12-6-4-5-10(2)9-12/h4-6,9,11H,3,7-8H2,1

InchiKey: XDTGDCZVKTYWSO-UHFFFAOYSA-N

Formula: C13H17NO

SMILES: CCN(C(=O)C1CC1)c1cccc(C)c1

Mol. weight [g/mol]: 203.28

Physical Properties

Property code	Value	Unit	Source
gf	203.97	kJ/mol	Joback Method
hf	-58.84	kJ/mol	Joback Method
hfus	25.83	kJ/mol	Joback Method
hvap	56.17	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.758		Crippen Method
mcvol	170.960	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
rinpol	1584.00		NIST Webbook
rinpol	1584.00		NIST Webbook
tb	601.55	K	Joback Method
tc	819.00	K	Joback Method
tf	375.55	K	Joback Method
vc	0.636	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.49	J/mol×K	601.55	Joback Method
cpg	456.47	J/mol×K	637.79	Joback Method
cpg	472.29	J/mol×K	674.03	Joback Method
cpg	487.03	J/mol×K	710.27	Joback Method
cpg	500.77	J/mol×K	746.52	Joback Method
cpg	513.57	J/mol×K	782.76	Joback Method
cpg	525.53	J/mol×K	819.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308576&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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