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

Inchi: InChI=1S/C16H23NO/c1-3-17(15-11-7-8-13(2)12-15)16(18)14-9-5-4-6-10-14/h7-8,11-12,

InchiKey: NARFYVMKRROFNU-UHFFFAOYSA-N

Formula: C16H23NO

SMILES: CCN(C(=O)C1CCCCC1)c1cccc(C)c1

Mol. weight [g/mol]: 245.36

Physical Properties

Property code	Value	Unit	Source
gf	192.93	kJ/mol	Joback Method
hf	-139.24	kJ/mol	Joback Method
hfus	27.30	kJ/mol	Joback Method
hvap	63.37	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.928		Crippen Method
mcvol	213.230	ml/mol	McGowan Method
pc	2119.73	kPa	Joback Method
rinpol	1823.00		NIST Webbook
tb	683.00	K	Joback Method
tc	909.69	K	Joback Method
tf	398.80	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.53	J/mol×K	683.00	Joback Method
cpg	625.00	J/mol×K	720.78	Joback Method
cpg	643.99	J/mol×K	758.56	Joback Method
cpg	661.59	J/mol×K	796.34	Joback Method
cpg	677.86	J/mol×K	834.12	Joback Method
cpg	692.87	J/mol×K	871.90	Joback Method
cpg	706.69	J/mol×K	909.69	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308520&Units=SI

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