N-Ethyl-N-methyl-benzamide

Inchi: InChI=1S/C10H13NO/c1-3-11(2)10(12)9-7-5-4-6-8-9/h4-8H,3H2,1-2H3
InchiKey: YPHRECOHXALQKL-UHFFFAOYSA-N
Formula: C10H13NO
SMILES: CCN(C)C(=O)c1ccccc1
Mol. weight [g/mol]: 163.22

Physical Properties

Property code	Value	Unit	Source
gf	127.59	kJ/mol	Joback Method
hf	-58.25	kJ/mol	Joback Method
hfus	20.32	kJ/mol	Joback Method
hvap	48.92	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	1.779		Crippen Method
mcvol	139.550	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
rinpol	1459.87		NIST Webbook
rinpol	1482.20		NIST Webbook
rinpol	1461.71		NIST Webbook
rinpol	1439.62		NIST Webbook
rinpol	1439.62		NIST Webbook
ripol	2370.92		NIST Webbook
ripol	2391.82		NIST Webbook
ripol	2412.54		NIST Webbook
ripol	2370.92		NIST Webbook
tb	521.19	K	Joback Method
tc	732.99	K	Joback Method
tf	311.28	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.15	J/mol×K	521.19	Joback Method

cpg	324.85	J/mol×K	556.49	Joback Method
cpg	338.60	J/mol×K	591.79	Joback Method
cpg	351.47	J/mol×K	627.09	Joback Method
cpg	363.49	J/mol×K	662.39	Joback Method
cpg	374.69	J/mol×K	697.69	Joback Method
cpg	385.14	J/mol×K	732.99	Joback Method

Sources

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=R194126&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume