N-Heptyl-N-methyl-benzamide

Inchi: InChI=1S/C15H23NO/c1-3-4-5-6-10-13-16(2)15(17)14-11-8-7-9-12-14/h7-9,11-12H,3-6,1
InchiKey: FCTHNQAPXOSDJH-UHFFFAOYSA-N
Formula: C15H23NO
SMILES: CCCCCCCN(C)C(=O)c1ccccc1
Mol. weight [g/mol]: 233.35

Physical Properties

Property code	Value	Unit	Source
gf	169.69	kJ/mol	Joback Method
hf	-161.45	kJ/mol	Joback Method
hfus	33.27	kJ/mol	Joback Method
hvap	60.05	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.729		Crippen Method
mcvol	210.000	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
rinpol	1902.92		NIST Webbook
rinpol	1904.96		NIST Webbook
rinpol	1925.16		NIST Webbook
rinpol	1882.54		NIST Webbook
ripol	2835.23		NIST Webbook
ripol	2815.37		NIST Webbook
ripol	2856.14		NIST Webbook
tb	635.59	K	Joback Method
tc	832.38	K	Joback Method
tf	367.63	K	Joback Method
vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.20	J/mol×K	635.59	Joback Method
cpg	574.64	J/mol×K	668.39	Joback Method
cpg	591.06	J/mol×K	701.19	Joback Method

cpg	606.51	J/mol×K	733.98	Joback Method
cpg	621.04	J/mol×K	766.78	Joback Method
cpg	634.68	J/mol×K	799.58	Joback Method
cpg	647.49	J/mol×K	832.38	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=R194131&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