Benzamide, 4-methyl-N-octyl-

Inchi: InChI=1S/C16H25NO/c1-3-4-5-6-7-8-13-17-16(18)15-11-9-14(2)10-12-15/h9-12H,3-8,13
InchiKey: YLOQYJXWAPFPMJ-UHFFFAOYSA-N
Formula: C16H25NO
SMILES: CCCCCCCCNC(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 247.38

Physical Properties

Property code	Value	Unit	Source
gf	147.09	kJ/mol	Joback Method
hf	-207.62	kJ/mol	Joback Method
hfus	37.55	kJ/mol	Joback Method
hvap	67.33	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.085		Crippen Method
mcvol	224.090	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
rinpol	2215.00		NIST Webbook
rinpol	2215.00		NIST Webbook
tb	701.18	K	Joback Method
tc	899.50	K	Joback Method
tf	411.61	K	Joback Method
vc	0.865	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.30	J/mol×K	701.18	Joback Method
cpg	646.06	J/mol×K	734.23	Joback Method
cpg	661.86	J/mol×K	767.29	Joback Method
cpg	676.73	J/mol×K	800.34	Joback Method
cpg	690.72	J/mol×K	833.40	Joback Method
cpg	703.86	J/mol×K	866.45	Joback Method
cpg	716.19	J/mol×K	899.50	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=U407473&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume