Benzamide, N-(3-methylphenyl)-4-butyl-

Inchi: InChI=1S/C18H21NO/c1-3-4-7-15-9-11-16(12-10-15)18(20)19-17-8-5-6-14(2)13-17/h5-6,
InchiKey: RBGTWZGRJGRVJU-UHFFFAOYSA-N
Formula: C18H21NO
SMILES: CCCCc1ccc(C(=O)Nc2cccc(C)c2)cc1
Mol. weight [g/mol]: 267.37

Physical Properties

Property code	Value	Unit	Source
gf	266.71	kJ/mol	Joback Method
hf	-23.84	kJ/mol	Joback Method
hfus	36.38	kJ/mol	Joback Method
hvap	74.72	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	4.590		Crippen Method
mcvol	228.510	ml/mol	McGowan Method
pc	1996.55	kPa	Joback Method
rinpol	2506.00		NIST Webbook
tb	778.60	K	Joback Method
tc	1006.16	K	Joback Method
tf	473.09	K	Joback Method
vc	0.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.09	J/mol×K	778.60	Joback Method
cpg	669.04	J/mol×K	816.53	Joback Method
cpg	683.80	J/mol×K	854.45	Joback Method
cpg	697.46	J/mol×K	892.38	Joback Method
cpg	710.07	J/mol×K	930.31	Joback Method
cpg	721.70	J/mol×K	968.23	Joback Method
cpg	732.43	J/mol×K	1006.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306991&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

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