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

Inchi: InChI=1S/C16H25NO/c1-4-5-6-14-7-9-15(10-8-14)16(18)17-12-11-13(2)3/h7-10,13H,4-6
InchiKey: HUYRCYTUDIKIJF-UHFFFAOYSA-N
Formula: C16H25NO
SMILES: CCCCc1ccc(C(=O)NCCC(C)C)cc1
Mol. weight [g/mol]: 247.38

Physical Properties

Property code	Value	Unit	Source
gf	144.65	kJ/mol	Joback Method
hf	-212.90	kJ/mol	Joback Method
hfus	34.02	kJ/mol	Joback Method
hvap	66.94	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	3.805		Crippen Method
mcvol	224.090	ml/mol	McGowan Method
pc	1804.63	kPa	Joback Method
rinpol	2158.00		NIST Webbook
rinpol	2158.00		NIST Webbook
tb	700.74	K	Joback Method
tc	902.26	K	Joback Method
tf	396.61	K	Joback Method
vc	0.859	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.79	J/mol×K	700.74	Joback Method
cpg	646.85	J/mol×K	734.33	Joback Method
cpg	662.90	J/mol×K	767.91	Joback Method
cpg	677.99	J/mol×K	801.50	Joback Method
cpg	692.15	J/mol×K	835.09	Joback Method
cpg	705.43	J/mol×K	868.68	Joback Method
cpg	717.87	J/mol×K	902.26	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=U407449&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