Benzamide, N-(3-methylbutyl)

Inchi: InChI=1S/C12H17NO/c1-10(2)8-9-13-12(14)11-6-4-3-5-7-11/h3-7,10H,8-9H2,1-2H3,(H,1
InchiKey: PMBAZUADXYLDHV-UHFFFAOYSA-N
Formula: C12H17NO
SMILES: CC(C)CCNC(=O)c1ccccc1
Mol. weight [g/mol]: 191.27

Physical Properties

Property code	Value	Unit	Source
gf	120.60	kJ/mol	Joback Method
hf	-118.87	kJ/mol	Joback Method
hfus	24.05	kJ/mol	Joback Method
hvap	57.38	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.462		Crippen Method
mcvol	167.730	ml/mol	McGowan Method
pc	2616.41	kPa	Joback Method
rinpol	1677.00		NIST Webbook
rinpol	1677.00		NIST Webbook
tb	604.24	K	Joback Method
tc	816.64	K	Joback Method
tf	339.01	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.45	J/mol×K	604.24	Joback Method
cpg	436.03	J/mol×K	639.64	Joback Method
cpg	450.64	J/mol×K	675.04	Joback Method
cpg	464.30	J/mol×K	710.44	Joback Method
cpg	477.08	J/mol×K	745.84	Joback Method
cpg	489.00	J/mol×K	781.24	Joback Method
cpg	500.11	J/mol×K	816.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R323087&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