

Benzoic acid, 2-(3-methylbutyl)amino-, 3-methylbutyl ester

Inchi:	InChI=1S/C17H27NO2/c1-13(2)9-11-18-16-8-6-5-7-15(16)17(19)20-12-10-14(3)4/h5-8,10
InchiKey:	JVOIWHLNJGEFLE-UHFFFAOYSA-N
Formula:	C17H27NO2
SMILES:	CC(C)CCNc1cccc1C(=O)OCCC(C)C
Mol. weight [g/mol]:	277.40

Physical Properties

Property code	Value	Unit	Source
gf	45.63	kJ/mol	Joback Method
hf	-371.04	kJ/mol	Joback Method
hfus	34.28	kJ/mol	Joback Method
hvap	71.19	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.348		Crippen Method
mvol	244.050	ml/mol	McGowan Method
pc	1653.80	kPa	Joback Method
rinpol	2053.00		NIST Webbook
rinpol	2053.00		NIST Webbook
tb	745.60	K	Joback Method
tc	947.13	K	Joback Method
tf	415.11	K	Joback Method
vc	0.926	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.08	J/molxK	745.60	Joback Method
cpg	732.26	J/molxK	779.19	Joback Method
cpg	748.38	J/molxK	812.78	Joback Method
cpg	763.48	J/molxK	846.36	Joback Method
cpg	777.58	J/molxK	879.95	Joback Method
cpg	790.71	J/molxK	913.54	Joback Method
cpg	802.91	J/molxK	947.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375470&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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