

4-Butylbenzoic acid, 3-methylbutyl ester

Inchi:	InChI=1S/C16H24O2/c1-4-5-6-14-7-9-15(10-8-14)16(17)18-12-11-13(2)3/h7-10,13H,4-6,
InchiKey:	XFLZSMLNZLATFX-UHFFFAOYSA-N
Formula:	C16H24O2
SMILES:	CCCCc1ccc(C(=O)OCCC(C)C)cc1
Mol. weight [g/mol]:	248.36

Physical Properties

Property code	Value	Unit	Source
gf	-49.74	kJ/mol	Joback Method
hf	-398.59	kJ/mol	Joback Method
hfus	30.11	kJ/mol	Joback Method
hvap	62.92	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.232		Crippen Method
mvol	219.980	ml/mol	McGowan Method
pc	1759.49	kPa	Joback Method
rinpol	1919.00		NIST Webbook
rinpol	1919.00		NIST Webbook
tb	672.99	K	Joback Method
tc	872.43	K	Joback Method
tf	366.18	K	Joback Method
vc	0.842	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.19	J/molxK	672.99	Joback Method
cpg	617.51	J/molxK	706.23	Joback Method
cpg	633.87	J/molxK	739.47	Joback Method
cpg	649.27	J/molxK	772.71	Joback Method
cpg	663.76	J/molxK	805.95	Joback Method
cpg	677.35	J/molxK	839.19	Joback Method
cpg	690.07	J/molxK	872.43	Joback Method
dvisc	0.0017472	Paxs	366.18	Joback Method

dvisc	0.0008353	Paxs	417.31	Joback Method
dvisc	0.0004692	Paxs	468.45	Joback Method
dvisc	0.0002952	Paxs	519.59	Joback Method
dvisc	0.0002018	Paxs	570.72	Joback Method
dvisc	0.0001469	Paxs	621.86	Joback Method
dvisc	0.0001122	Paxs	672.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354163&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
mccvol:	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

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