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
mcvol	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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0008353	Pa×s	417.31	Joback Method
dvisc	0.0004692	Pa×s	468.45	Joback Method
dvisc	0.0002952	Pa×s	519.59	Joback Method
dvisc	0.0002018	Pa×s	570.72	Joback Method
dvisc	0.0001469	Pa×s	621.86	Joback Method
dvisc	0.0001122	Pa×s	672.99	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=U354163&Units=SI

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
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