4-Butylbenzoic acid, 2-methylpentyl ester

Inchi: InChI=1S/C17H26O2/c1-4-6-8-15-9-11-16(12-10-15)17(18)19-13-14(3)7-5-2/h9-12,14H,4
InchiKey: FAXLCUOSVAHYMS-UHFFFAOYSA-N
Formula: C17H26O2
SMILES: CCCCc1ccc(C(=O)OCC(C)CCC)cc1
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	-41.32	kJ/mol	Joback Method
hf	-419.23	kJ/mol	Joback Method
hfus	32.70	kJ/mol	Joback Method
hvap	65.14	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.622		Crippen Method
mcvol	234.070	ml/mol	McGowan Method
pc	1625.91	kPa	Joback Method
rinpol	2009.00		NIST Webbook
tb	695.87	K	Joback Method
tc	893.18	K	Joback Method
tf	377.45	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.09	J/mol×K	695.87	Joback Method
cpg	672.74	J/mol×K	728.76	Joback Method
cpg	689.39	J/mol×K	761.64	Joback Method
cpg	705.08	J/mol×K	794.53	Joback Method
cpg	719.83	J/mol×K	827.41	Joback Method
cpg	733.66	J/mol×K	860.30	Joback Method
cpg	746.60	J/mol×K	893.18	Joback Method
dvisc	0.0016219	Pa×s	377.45	Joback Method
dvisc	0.0007654	Pa×s	430.52	Joback Method

dvisc	0.0004259	Pa×s	483.59	Joback Method
dvisc	0.0002661	Pa×s	536.66	Joback Method
dvisc	0.0001810	Pa×s	589.73	Joback Method
dvisc	0.0001312	Pa×s	642.80	Joback Method
dvisc	0.0000999	Pa×s	695.87	Joback Method

Sources

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=U354165&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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