4-Butylbenzoic acid, 3-methylphenyl ester

Inchi: InChI=1S/C18H20O2/c1-3-4-7-15-9-11-16(12-10-15)18(19)20-17-8-5-6-14(2)13-17/h5-6,
InchiKey: JRMTVKFNYIYFDG-UHFFFAOYSA-N
Formula: C18H20O2
SMILES: CCCCc1ccc(C(=O)Oc2cccc(C)c2)cc1
Mol. weight [g/mol]: 268.35

Physical Properties

Property code	Value	Unit	Source
gf	72.32	kJ/mol	Joback Method
hf	-209.53	kJ/mol	Joback Method
hfus	32.47	kJ/mol	Joback Method
hvap	70.69	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.557		Crippen Method
mcvol	224.400	ml/mol	McGowan Method
pc	1944.08	kPa	Joback Method
rinpol	2182.00		NIST Webbook
rinpol	2182.00		NIST Webbook
tb	750.85	K	Joback Method
tc	977.15	K	Joback Method
tf	442.66	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.01	J/mol×K	750.85	Joback Method
cpg	641.41	J/mol×K	788.57	Joback Method
cpg	656.60	J/mol×K	826.28	Joback Method
cpg	670.63	J/mol×K	864.00	Joback Method
cpg	683.56	J/mol×K	901.72	Joback Method
cpg	695.42	J/mol×K	939.44	Joback Method
cpg	706.26	J/mol×K	977.15	Joback Method
dvisc	0.0008527	Pa×s	442.66	Joback Method

dvisc	0.0004924	Pa×s	494.03	Joback Method
dvisc	0.0003153	Pa×s	545.39	Joback Method
dvisc	0.0002180	Pa×s	596.75	Joback Method
dvisc	0.0001598	Pa×s	648.12	Joback Method
dvisc	0.0001226	Pa×s	699.49	Joback Method
dvisc	0.0000976	Pa×s	750.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307503&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
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
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

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