4-Butylbenzoic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C19H22O2/c1-4-5-6-16-7-9-17(10-8-16)19(20)21-18-12-14(2)11-15(3)13-18/h7
InchiKey: XASPIHMVPNXWQD-UHFFFAOYSA-N
Formula: C19H22O2
SMILES: CCCCc1ccc(C(=O)Oc2cc(C)cc(C)c2)cc1
Mol. weight [g/mol]: 282.38

Physical Properties

Property code	Value	Unit	Source
gf	71.11	kJ/mol	Joback Method
hf	-241.64	kJ/mol	Joback Method
hfus	34.67	kJ/mol	Joback Method
hvap	73.58	kJ/mol	Joback Method
log10ws	-6.15		Crippen Method
logp	4.865		Crippen Method
mcvol	238.490	ml/mol	McGowan Method
pc	1766.90	kPa	Joback Method
rinpol	2291.00		NIST Webbook
rinpol	2291.00		NIST Webbook
tb	778.71	K	Joback Method
tc	1002.35	K	Joback Method
tf	466.45	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.82	J/mol×K	778.71	Joback Method
cpg	750.66	J/mol×K	965.07	Joback Method
cpg	738.72	J/mol×K	927.80	Joback Method
cpg	725.70	J/mol×K	890.53	Joback Method
cpg	711.58	J/mol×K	853.26	Joback Method
cpg	696.29	J/mol×K	815.98	Joback Method
cpg	761.56	J/mol×K	1002.35	Joback Method
dvisc	0.0000874	Pa×s	778.71	Joback Method

dvisc	0.0001088	Pa×s	726.67	Joback Method
dvisc	0.0001400	Pa×s	674.62	Joback Method
dvisc	0.0001881	Pa×s	622.58	Joback Method
dvisc	0.0002666	Pa×s	570.54	Joback Method
dvisc	0.0004053	Pa×s	518.49	Joback Method
dvisc	0.0006765	Pa×s	466.45	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=U307505&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