4-Butylbenzoic acid, 2-propylphenyl ester

Inchi: InChI=1S/C20H24O2/c1-3-5-9-16-12-14-18(15-13-16)20(21)22-19-11-7-6-10-17(19)8-4-2
InchiKey: FUHJNUGUFXFGCO-UHFFFAOYSA-N
Formula: C20H24O2
SMILES: CCCCc1ccc(C(=O)Oc2ccccc2CCC)cc1
Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	89.16	kJ/mol	Joback Method
hf	-250.81	kJ/mol	Joback Method
hfus	37.65	kJ/mol	Joback Method
hvap	75.15	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	5.201		Crippen Method
mcvol	252.580	ml/mol	McGowan Method
pc	1652.46	kPa	Joback Method
rinpol	2391.00		NIST Webbook
tb	796.61	K	Joback Method
tc	1016.59	K	Joback Method
tf	465.20	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.27	J/mol×K	796.61	Joback Method
cpg	754.01	J/mol×K	833.27	Joback Method
cpg	769.54	J/mol×K	869.94	Joback Method
cpg	783.90	J/mol×K	906.60	Joback Method
cpg	797.14	J/mol×K	943.26	Joback Method
cpg	809.31	J/mol×K	979.93	Joback Method
cpg	820.46	J/mol×K	1016.59	Joback Method
dvisc	0.0007341	Pa×s	465.20	Joback Method
dvisc	0.0004125	Pa×s	520.44	Joback Method

dvisc	0.0002589	Pa×s	575.67	Joback Method
dvisc	0.0001763	Pa×s	630.90	Joback Method
dvisc	0.0001277	Pa×s	686.14	Joback Method
dvisc	0.0000971	Pa×s	741.38	Joback Method
dvisc	0.0000767	Pa×s	796.61	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=U354321&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