4-Butylbenzoic acid, 2-naphthyl ester

Inchi: InChI=1S/C21H20O2/c1-2-3-6-16-9-11-18(12-10-16)21(22)23-20-14-13-17-7-4-5-8-19(17
InchiKey: DIGPSVUCITZYQS-UHFFFAOYSA-N
Formula: C21H20O2
SMILES: CCCCc1ccc(C(=O)Oc2ccc3ccccc3c2)cc1
Mol. weight [g/mol]: 304.38

Physical Properties

Property code	Value	Unit	Source
gf	204.23	kJ/mol	Joback Method
hf	-80.38	kJ/mol	Joback Method
hfus	37.26	kJ/mol	Joback Method
hvap	79.01	kJ/mol	Joback Method
log10ws	-7.00		Crippen Method
logp	5.402		Crippen Method
mcvol	247.210	ml/mol	McGowan Method
pc	1872.41	kPa	Joback Method
rinpol	2710.00		NIST Webbook
rinpol	2710.00		NIST Webbook
tb	838.47	K	Joback Method
tc	1076.75	K	Joback Method
tf	509.17	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.93	J/mol×K	838.47	Joback Method
cpg	786.74	J/mol×K	1037.04	Joback Method
cpg	775.56	J/mol×K	997.32	Joback Method
cpg	763.49	J/mol×K	957.61	Joback Method
cpg	750.43	J/mol×K	917.90	Joback Method
cpg	736.27	J/mol×K	878.18	Joback Method
cpg	797.11	J/mol×K	1076.75	Joback Method
dvisc	0.0001327	Pa×s	838.47	Joback Method

dvisc	0.0001611	Pa×s	783.59	Joback Method
dvisc	0.0002014	Pa×s	728.70	Joback Method
dvisc	0.0002611	Pa×s	673.82	Joback Method
dvisc	0.0003545	Pa×s	618.94	Joback Method
dvisc	0.0005108	Pa×s	564.05	Joback Method
dvisc	0.0007962	Pa×s	509.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307510&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