N-butyl-o-benzoyl benzoate

Inchi: InChI=1S/C18H18O3/c1-2-3-13-21-18(20)16-12-8-7-11-15(16)17(19)14-9-5-4-6-10-14/h4
InchiKey: VMHKPGQWBDCKSM-UHFFFAOYSA-N
Formula: C18H18O3
SMILES: CCCCOC(=O)c1ccccc1C(=O)c1ccccc1
Mol. weight [g/mol]: 282.33
CAS: 571-98-2

Physical Properties

Property code	Value	Unit	Source
gf	-46.97	kJ/mol	Joback Method
hf	-310.64	kJ/mol	Joback Method
hfus	34.45	kJ/mol	Joback Method
hvap	76.78	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	3.874		Crippen Method
mcvol	225.970	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
tb	799.74	K	Joback Method
tc	1030.70	K	Joback Method
tf	480.07	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.46	J/mol×K	799.74	Joback Method
cpg	655.99	J/mol×K	838.23	Joback Method
cpg	669.31	J/mol×K	876.73	Joback Method
cpg	681.46	J/mol×K	915.22	Joback Method
cpg	692.51	J/mol×K	953.71	Joback Method
cpg	702.51	J/mol×K	992.20	Joback Method
cpg	711.51	J/mol×K	1030.70	Joback Method
dvisc	0.0008645	Pa×s	480.07	Joback Method
dvisc	0.0004996	Pa×s	533.35	Joback Method

dvisc	0.0003189	Pa×s	586.63	Joback Method
dvisc	0.0002194	Pa×s	639.90	Joback Method
dvisc	0.0001599	Pa×s	693.18	Joback Method
dvisc	0.0001219	Pa×s	746.46	Joback Method
dvisc	0.0000963	Pa×s	799.74	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=C571982&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume