4-Butylbenzoic acid, 2-adamantyl ester

Inchi: InChI=1S/C21H28O2/c1-2-3-4-14-5-7-17(8-6-14)21(22)23-20-18-10-15-9-16(12-18)13-19
InchiKey: XPXKHQKPWRXECF-UHFFFAOYSA-N
Formula: C21H28O2
SMILES: CCCCc1ccc(C(=O)OC2C3CC4CC(C3)CC2C4)cc1
Mol. weight [g/mol]: 312.45

Physical Properties

Property code	Value	Unit	Source
gf	149.53	kJ/mol	Joback Method
hf	-324.95	kJ/mol	Joback Method
hfus	41.03	kJ/mol	Joback Method
hvap	73.73	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.011		Crippen Method
mcvol	257.850	ml/mol	McGowan Method
pc	1570.96	kPa	Joback Method
rinpol	2462.40		NIST Webbook
tb	802.98	K	Joback Method
tc	1025.82	K	Joback Method
tf	479.35	K	Joback Method
vc	0.989	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.28	J/mol×K	802.98	Joback Method
cpg	868.71	J/mol×K	840.12	Joback Method
cpg	887.81	J/mol×K	877.26	Joback Method
cpg	905.71	J/mol×K	914.40	Joback Method
cpg	922.52	J/mol×K	951.54	Joback Method
cpg	938.35	J/mol×K	988.68	Joback Method
cpg	953.34	J/mol×K	1025.82	Joback Method
dvisc	0.0039208	Pa×s	479.35	Joback Method
dvisc	0.0033058	Pa×s	533.29	Joback Method

dvisc	0.0028759	Pa×s	587.23	Joback Method
dvisc	0.0025613	Pa×s	641.16	Joback Method
dvisc	0.0023225	Pa×s	695.10	Joback Method
dvisc	0.0021359	Pa×s	749.04	Joback Method
dvisc	0.0019864	Pa×s	802.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292207&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