4-Butylbenzoic acid, 2-(1-adamantyl)ethyl ester

Inchi: InChI=1S/C23H32O2/c1-2-3-4-17-5-7-21(8-6-17)22(24)25-10-9-23-14-18-11-19(15-23)13

InchiKey: USHJKDDEMUOFQR-UHFFFAOYSA-N

Formula: C23H32O2

SMILES: CCCCc1ccc(C(=O)OCCC23CC4CC(CC(C4)C2)C3)cc1

Mol. weight [g/mol]: 340.50

Physical Properties

Property code	Value	Unit	Source
gf	168.59	kJ/mol	Joback Method
hf	-330.65	kJ/mol	Joback Method
hfus	38.84	kJ/mol	Joback Method
hvap	77.34	kJ/mol	Joback Method
log10ws	-6.68		Crippen Method
logp	5.793		Crippen Method
mcvol	286.030	ml/mol	McGowan Method
pc	1438.07	kPa	Joback Method
rinpol	2622.70		NIST Webbook
rinpol	2622.70		NIST Webbook
tb	853.65	K	Joback Method
tc	1077.58	K	Joback Method
tf	530.03	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	962.02	J/mol×K	853.65	Joback Method
cpg	984.18	J/mol×K	890.97	Joback Method
cpg	1005.84	J/mol×K	928.29	Joback Method
cpg	1027.21	J/mol×K	965.62	Joback Method
cpg	1048.54	J/mol×K	1002.94	Joback Method
cpg	1070.04	J/mol×K	1040.26	Joback Method
cpg	1091.96	J/mol×K	1077.58	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=U292209&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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