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]: 340.51

Physical Properties

Property code	Value	Unit	Source
af	0.7928		Cheméo Relay (1.0)
hfus	38.84	kJ/mol	Joback Method
log10ws	-7.03		Cheméo Relay (1.0)
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	694.95	K	Cheméo Relay (1.0)
tc	946.60	K	Cheméo Relay (1.0)
tf	406.46	K	Cheméo Relay (1.0)
vc	1.059	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292209&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion 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