4-Butylbenzoic acid, 1-adamantylmethyl ester

Inchi: InChI=1S/C22H30O2/c1-2-3-4-16-5-7-20(8-6-16)21(23)24-15-22-12-17-9-18(13-22)11-19
InchiKey: OFLCWOOKKFWXER-UHFFFAOYSA-N
Formula: C22H30O2
SMILES: CCCCc1ccc(C(=O)OCC23CC4CC(CC(C4)C2)C3)cc1
Mol. weight [g/mol]: 326.47

Physical Properties

Property code	Value	Unit	Source
gf	160.17	kJ/mol	Joback Method
hf	-310.01	kJ/mol	Joback Method
hfus	36.25	kJ/mol	Joback Method
hvap	75.11	kJ/mol	Joback Method
log10ws	-6.26		Crippen Method
logp	5.402		Crippen Method
mcvol	271.940	ml/mol	McGowan Method
pc	1548.78	kPa	Joback Method
rinpol	2533.80		NIST Webbook
rinpol	2533.80		NIST Webbook
tb	830.77	K	Joback Method
tc	1057.09	K	Joback Method
tf	518.76	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	900.79	J/mol×K	830.77	Joback Method
cpg	922.55	J/mol×K	868.49	Joback Method
cpg	943.71	J/mol×K	906.21	Joback Method
cpg	964.51	J/mol×K	943.93	Joback Method
cpg	985.19	J/mol×K	981.65	Joback Method
cpg	1005.96	J/mol×K	1019.37	Joback Method
cpg	1027.08	J/mol×K	1057.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292208&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

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

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