1-Adamantanecarboxylic acid , 4-benzyloxyphenyl ester

Inchi: InChI=1S/C24H26O3/c25-23(24-13-18-10-19(14-24)12-20(11-18)15-24)27-22-8-6-21(7-9

InchiKey: WUJQQYJSAUMYHW-UHFFFAOYSA-N

Formula: C24H26O3

SMILES: O=C(Oc1ccc(OCc2ccccc2)cc1)C12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 362.46

Physical Properties

Property code	Value	Unit	Source
gf	184.42	kJ/mol	Joback Method
hf	-246.98	kJ/mol	Joback Method
hfus	36.66	kJ/mol	Joback Method
hvap	84.25	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	5.387		Crippen Method
mcvol	282.230	ml/mol	McGowan Method
pc	1708.95	kPa	Joback Method
rinpol	3170.00		NIST Webbook
rinpol	3170.00		NIST Webbook
tb	925.63	K	Joback Method
tc	1177.11	K	Joback Method
tf	589.95	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	959.34	J/mol×K	925.63	Joback Method
cpg	981.43	J/mol×K	967.54	Joback Method
cpg	1003.38	J/mol×K	1009.46	Joback Method
cpg	1025.51	J/mol×K	1051.37	Joback Method
cpg	1048.14	J/mol×K	1093.29	Joback Method
cpg	1071.59	J/mol×K	1135.20	Joback Method
cpg	1096.18	J/mol×K	1177.11	Joback Method

Sources

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=U307667&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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