Isophthalic acid, 1-adamantylmethyl isobutyl ester

Inchi: InChI=1S/C23H30O4/c1-15(2)13-26-21(24)19-4-3-5-20(9-19)22(25)27-14-23-10-16-6-17(11-23)8-18(7-16)12-23/h3-5,9,15-18H,6-8,10-14H2,1-2H3

InchiKey: UTFVDGIJHSHNQO-UHFFFAOYSA-N

Formula: C23H30O4

SMILES: CC(C)COC(=O)c1cccc(C(=O)OCC23CC4CC(CC(C4)C2)C3)c1

Mol. weight [g/mol]: 370.48

Physical Properties

Property code	Value	Unit	Source
gf	-67.77	kJ/mol	Joback Method
hf	-580.73	kJ/mol	Joback Method
hfus	38.11	kJ/mol	Joback Method
hvap	86.10	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	4.873		Crippen Method
mcvol	293.470	ml/mol	McGowan Method
pc	1498.83	kPa	Joback Method
rinpol	2982.00		NIST Webbook
rinpol	2982.00		NIST Webbook
tb	929.50	K	Joback Method
tc	1161.37	K	Joback Method
tf	587.19	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1016.06	J/mol×K	929.50	Joback Method
cpg	1037.45	J/mol×K	968.15	Joback Method
cpg	1058.63	J/mol×K	1006.79	Joback Method
cpg	1079.81	J/mol×K	1045.44	Joback Method
cpg	1101.25	J/mol×K	1084.08	Joback Method
cpg	1123.17	J/mol×K	1122.73	Joback Method
cpg	1145.80	J/mol×K	1161.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343962&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