Isophthalic acid, 1-adamantylmethyl pentyl ester

Inchi: InChI=1S/C24H32O4/c1-2-3-4-8-27-22(25)20-6-5-7-21(12-20)23(26)28-16-24-13-17-9-18

InchiKey: ZEBLMXVQRGBIQK-UHFFFAOYSA-N

Formula: C24H32O4

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

Mol. weight [g/mol]: 384.51

Physical Properties

Property code	Value	Unit	Source
gf	-56.91	kJ/mol	Joback Method
hf	-596.09	kJ/mol	Joback Method
hfus	44.22	kJ/mol	Joback Method
hvap	88.72	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	5.407		Crippen Method
mcvol	307.560	ml/mol	McGowan Method
pc	1385.05	kPa	Joback Method
rinpol	3142.00		NIST Webbook
rinpol	3142.00		NIST Webbook
tb	952.82	K	Joback Method
tc	1181.60	K	Joback Method
tf	613.46	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1078.90	J/mol×K	952.82	Joback Method
cpg	1100.80	J/mol×K	990.95	Joback Method
cpg	1122.57	J/mol×K	1029.08	Joback Method
cpg	1144.44	J/mol×K	1067.21	Joback Method
cpg	1166.66	J/mol×K	1105.34	Joback Method
cpg	1189.44	J/mol×K	1143.47	Joback Method
cpg	1213.01	J/mol×K	1181.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343964&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