Isophthalic acid, 1-adamantylmethyl octyl ester

Inchi: InChI=1S/C27H38O4/c1-2-3-4-5-6-7-11-30-25(28)23-9-8-10-24(15-23)26(29)31-19-27-16

InchiKey: ZBIFSFGFTFIBOJ-UHFFFAOYSA-N

Formula: C27H38O4

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

Mol. weight [g/mol]: 426.59

Physical Properties

Property code	Value	Unit	Source
gf	-31.65	kJ/mol	Joback Method
hf	-658.01	kJ/mol	Joback Method
hfus	51.99	kJ/mol	Joback Method
hvap	95.40	kJ/mol	Joback Method
log10ws	-7.79		Crippen Method
logp	6.577		Crippen Method
mcvol	349.830	ml/mol	McGowan Method
pc	1129.86	kPa	Joback Method
rinpol	3452.00		NIST Webbook
rinpol	3452.00		NIST Webbook
tb	1021.46	K	Joback Method
tc	1253.72	K	Joback Method
tf	647.27	K	Joback Method
vc	1.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1274.37	J/mol×K	1021.46	Joback Method
cpg	1298.92	J/mol×K	1060.17	Joback Method
cpg	1323.62	J/mol×K	1098.88	Joback Method
cpg	1348.72	J/mol×K	1137.59	Joback Method
cpg	1374.48	J/mol×K	1176.30	Joback Method
cpg	1401.15	J/mol×K	1215.01	Joback Method
cpg	1428.98	J/mol×K	1253.72	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343968&Units=SI

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