Isophthalic acid, 1-adamantylmethyl isohexyl ester

Inchi: InChI=1S/C25H34O4/c1-17(2)5-4-8-28-23(26)21-6-3-7-22(12-21)24(27)29-16-25-13-18-9

InchiKey: QYQHZYYLENRCTN-UHFFFAOYSA-N

Formula: C25H34O4

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

Mol. weight [g/mol]: 398.54

Physical Properties

Property code	Value	Unit	Source
gf	-50.93	kJ/mol	Joback Method
hf	-622.01	kJ/mol	Joback Method
hfus	43.29	kJ/mol	Joback Method
hvap	90.56	kJ/mol	Joback Method
log10ws	-6.71		Crippen Method
logp	5.653		Crippen Method
mcvol	321.650	ml/mol	McGowan Method
pc	1298.60	kPa	Joback Method
rinpol	3204.00		NIST Webbook
rinpol	3204.00		NIST Webbook
tb	975.26	K	Joback Method
tc	1206.09	K	Joback Method
tf	609.73	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1143.44	J/mol×K	975.26	Joback Method
cpg	1166.20	J/mol×K	1013.73	Joback Method
cpg	1188.91	J/mol×K	1052.20	Joback Method
cpg	1211.81	J/mol×K	1090.67	Joback Method
cpg	1235.14	J/mol×K	1129.14	Joback Method
cpg	1259.12	J/mol×K	1167.61	Joback Method
cpg	1284.01	J/mol×K	1206.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343965&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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