Isophthalic acid, 1-adamantylmethyl butyl ester

Inchi: InChI=1S/C23H30O4/c1-2-3-7-26-21(24)19-5-4-6-20(11-19)22(25)27-15-23-12-16-8-17(1

InchiKey: YZWBHQYNVHQMAR-UHFFFAOYSA-N

Formula: C23H30O4

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

Mol. weight [g/mol]: 370.48

Physical Properties

Property code	Value	Unit	Source
gf	-65.33	kJ/mol	Joback Method
hf	-575.45	kJ/mol	Joback Method
hfus	41.63	kJ/mol	Joback Method
hvap	86.49	kJ/mol	Joback Method
log10ws	-6.12		Crippen Method
logp	5.017		Crippen Method
mcvol	293.470	ml/mol	McGowan Method
pc	1489.58	kPa	Joback Method
rinpol	3036.00		NIST Webbook
tb	929.94	K	Joback Method
tc	1159.29	K	Joback Method
tf	602.19	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1015.66	J/mol×K	929.94	Joback Method
cpg	1036.87	J/mol×K	968.16	Joback Method
cpg	1057.88	J/mol×K	1006.39	Joback Method
cpg	1078.92	J/mol×K	1044.61	Joback Method
cpg	1100.21	J/mol×K	1082.84	Joback Method
cpg	1121.98	J/mol×K	1121.06	Joback Method
cpg	1144.45	J/mol×K	1159.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343963&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