Isophthalic acid, 1-adamantylmethyl propyl ester

Inchi: InChI=1S/C22H28O4/c1-2-6-25-20(23)18-4-3-5-19(10-18)21(24)26-14-22-11-15-7-16(12

InchiKey: YFRRZWAZAJHLLZ-UHFFFAOYSA-N

Formula: C22H28O4

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

Mol. weight [g/mol]: 356.46

Physical Properties

Property code	Value	Unit	Source
gf	-73.75	kJ/mol	Joback Method
hf	-554.81	kJ/mol	Joback Method
hfus	39.04	kJ/mol	Joback Method
hvap	84.27	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	4.627		Crippen Method
mcvol	279.380	ml/mol	McGowan Method
pc	1606.42	kPa	Joback Method
rinpol	2914.00		NIST Webbook
rinpol	2914.00		NIST Webbook
tb	907.06	K	Joback Method
tc	1137.76	K	Joback Method
tf	590.92	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	953.39	J/mol×K	907.06	Joback Method
cpg	973.99	J/mol×K	945.51	Joback Method
cpg	994.33	J/mol×K	983.96	Joback Method
cpg	1014.61	J/mol×K	1022.41	Joback Method
cpg	1035.07	J/mol×K	1060.86	Joback Method
cpg	1055.93	J/mol×K	1099.31	Joback Method
cpg	1077.41	J/mol×K	1137.76	Joback Method

Sources

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=U343961&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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