Isophthalic acid, 1-adamantylmethyl hexyl ester

Inchi: InChI=1S/C25H34O4/c1-2-3-4-5-9-28-23(26)21-7-6-8-22(13-21)24(27)29-17-25-14-18-10

InchiKey: KCVPOSJGDLNQMP-UHFFFAOYSA-N

Formula: C25H34O4

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

Mol. weight [g/mol]: 398.54

Physical Properties

Property code	Value	Unit	Source
gf	-48.49	kJ/mol	Joback Method
hf	-616.73	kJ/mol	Joback Method
hfus	46.81	kJ/mol	Joback Method
hvap	90.94	kJ/mol	Joback Method
log10ws	-6.95		Crippen Method
logp	5.797		Crippen Method
mcvol	321.650	ml/mol	McGowan Method
pc	1291.14	kPa	Joback Method
rinpol	3247.00		NIST Webbook
rinpol	3247.00		NIST Webbook
tb	975.70	K	Joback Method
tc	1204.74	K	Joback Method
tf	624.73	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1143.12	J/mol×K	975.70	Joback Method
cpg	1165.77	J/mol×K	1013.87	Joback Method
cpg	1188.40	J/mol×K	1052.05	Joback Method
cpg	1211.22	J/mol×K	1090.22	Joback Method
cpg	1234.47	J/mol×K	1128.39	Joback Method
cpg	1258.38	J/mol×K	1166.57	Joback Method
cpg	1283.19	J/mol×K	1204.74	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=U343966&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