Phthalic acid, 5-ethyl-1,3-dioxan-5-yl heptyl ester

Inchi: InChI=1S/C22H32O6/c1-3-5-6-7-10-13-27-20(23)18-11-8-9-12-19(18)21(24)28-16-22(4-2

InchiKey: QXGGUADEGZIDGA-UHFFFAOYSA-N

Formula: C22H32O6

SMILES: CCCCCCCOC(=O)c1ccccc1C(=O)OCC1(CC)COCOC1

Mol. weight [g/mol]: 392.49

Physical Properties

Property code	Value	Unit	Source
gf	-383.98	kJ/mol	Joback Method
hf	-956.39	kJ/mol	Joback Method
hfus	53.46	kJ/mol	Joback Method
hvap	94.11	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	4.371		Crippen Method
mcvol	312.840	ml/mol	McGowan Method
pc	1381.96	kPa	Joback Method
rinpol	2986.00		NIST Webbook
rinpol	2986.00		NIST Webbook
tb	960.69	K	Joback Method
tc	1185.05	K	Joback Method
tf	605.38	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1059.42	J/mol×K	960.69	Joback Method
cpg	1078.30	J/mol×K	998.08	Joback Method
cpg	1096.55	J/mol×K	1035.48	Joback Method
cpg	1114.30	J/mol×K	1072.87	Joback Method
cpg	1131.69	J/mol×K	1110.26	Joback Method
cpg	1148.83	J/mol×K	1147.66	Joback Method
cpg	1165.87	J/mol×K	1185.05	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=U415483&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