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

Inchi: InChI=1S/C21H30O6/c1-3-5-6-9-12-26-19(22)17-10-7-8-11-18(17)20(23)27-15-21(4-2)13

InchiKey: QJTFIVPVBIEMKC-UHFFFAOYSA-N

Formula: C21H30O6

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

Mol. weight [g/mol]: 378.46

Physical Properties

Property code	Value	Unit	Source
gf	-392.40	kJ/mol	Joback Method
hf	-935.75	kJ/mol	Joback Method
hfus	50.87	kJ/mol	Joback Method
hvap	91.89	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.981		Crippen Method
mcvol	298.750	ml/mol	McGowan Method
pc	1486.14	kPa	Joback Method
rinpol	2886.00		NIST Webbook
rinpol	2886.00		NIST Webbook
tb	937.81	K	Joback Method
tc	1161.58	K	Joback Method
tf	594.11	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.35	J/mol×K	937.81	Joback Method
cpg	1015.74	J/mol×K	975.10	Joback Method
cpg	1033.49	J/mol×K	1012.40	Joback Method
cpg	1050.72	J/mol×K	1049.69	Joback Method
cpg	1067.54	J/mol×K	1086.99	Joback Method
cpg	1084.09	J/mol×K	1124.28	Joback Method
cpg	1100.49	J/mol×K	1161.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415482&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