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

Inchi: InChI=1S/C18H24O6/c1-3-9-23-16(19)14-7-5-6-8-15(14)17(20)24-12-18(4-2)10-21-13-22

InchiKey: ZMLOEDAYCZMNBY-UHFFFAOYSA-N

Formula: C18H24O6

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

Mol. weight [g/mol]: 336.38

Physical Properties

Property code	Value	Unit	Source
gf	-417.66	kJ/mol	Joback Method
hf	-873.83	kJ/mol	Joback Method
hfus	43.10	kJ/mol	Joback Method
hvap	85.21	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	2.811		Crippen Method
mcvol	256.480	ml/mol	McGowan Method
pc	1880.53	kPa	Joback Method
rinpol	2488.00		NIST Webbook
rinpol	2488.00		NIST Webbook
tb	869.17	K	Joback Method
tc	1095.89	K	Joback Method
tf	560.30	K	Joback Method
vc	0.957	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.23	J/mol×K	869.17	Joback Method
cpg	833.40	J/mol×K	906.96	Joback Method
cpg	849.85	J/mol×K	944.74	Joback Method
cpg	865.72	J/mol×K	982.53	Joback Method
cpg	881.10	J/mol×K	1020.31	Joback Method
cpg	896.13	J/mol×K	1058.10	Joback Method
cpg	910.92	J/mol×K	1095.89	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=U415478&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