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

Inchi: InChI=1S/C19H26O6/c1-4-19(10-22-13-23-11-19)12-25-18(21)16-8-6-5-7-15(16)17(20)2

InchiKey: YCAIDPAHEPLMIX-UHFFFAOYSA-N

Formula: C19H26O6

SMILES: CCC1(COC(=O)c2ccccc2C(=O)OCC(C)C)COCOC1

Mol. weight [g/mol]: 350.41

Physical Properties

Property code	Value	Unit	Source
gf	-411.68	kJ/mol	Joback Method
hf	-899.75	kJ/mol	Joback Method
hfus	42.16	kJ/mol	Joback Method
hvap	87.05	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.057		Crippen Method
mcvol	270.570	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
tb	891.61	K	Joback Method
tc	1119.33	K	Joback Method
tf	556.57	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	876.20	J/mol×K	891.61	Joback Method
cpg	893.93	J/mol×K	929.56	Joback Method
cpg	910.94	J/mol×K	967.52	Joback Method
cpg	927.35	J/mol×K	1005.47	Joback Method
cpg	943.28	J/mol×K	1043.42	Joback Method
cpg	958.86	J/mol×K	1081.38	Joback Method
cpg	974.22	J/mol×K	1119.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415479&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume