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

Inchi: InChI=1S/C19H26O6/c1-3-5-10-24-17(20)15-8-6-7-9-16(15)18(21)25-13-19(4-2)11-22-14
InchiKey: FQPAPVYQTHMASX-UHFFFAOYSA-N
Formula: C19H26O6
SMILES: CCCCOC(=O)c1ccccc1C(=O)OCC1(CC)COCOC1
Mol. weight [g/mol]: 350.41

Physical Properties

Property code	Value	Unit	Source
gf	-409.24	kJ/mol	Joback Method
hf	-894.47	kJ/mol	Joback Method
hfus	45.69	kJ/mol	Joback Method
hvap	87.44	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.201		Crippen Method
mcvol	270.570	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
rinpol	2682.00		NIST Webbook
rinpol	2682.00		NIST Webbook
tb	892.05	K	Joback Method
tc	1117.04	K	Joback Method
tf	571.57	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	875.71	J/mol×K	892.05	Joback Method
cpg	893.27	J/mol×K	929.55	Joback Method
cpg	910.13	J/mol×K	967.05	Joback Method
cpg	926.42	J/mol×K	1004.55	Joback Method
cpg	942.26	J/mol×K	1042.05	Joback Method
cpg	957.77	J/mol×K	1079.54	Joback Method
cpg	973.06	J/mol×K	1117.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415480&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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