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

Inchi: InChI=1S/C20H28O6/c1-3-5-8-11-25-18(21)16-9-6-7-10-17(16)19(22)26-14-20(4-2)12-23

InchiKey: CJKQETIMCSKERE-UHFFFAOYSA-N

Formula: C20H28O6

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

Mol. weight [g/mol]: 364.43

Physical Properties

Property code	Value	Unit	Source
gf	-400.82	kJ/mol	Joback Method
hf	-915.11	kJ/mol	Joback Method
hfus	48.28	kJ/mol	Joback Method
hvap	89.66	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.591		Crippen Method
mcvol	284.660	ml/mol	McGowan Method
pc	1602.56	kPa	Joback Method
rinpol	2782.00		NIST Webbook
rinpol	2782.00		NIST Webbook
tb	914.93	K	Joback Method
tc	1138.93	K	Joback Method
tf	582.84	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	936.10	J/mol×K	914.93	Joback Method
cpg	954.06	J/mol×K	952.26	Joback Method
cpg	971.35	J/mol×K	989.60	Joback Method
cpg	988.09	J/mol×K	1026.93	Joback Method
cpg	1004.41	J/mol×K	1064.26	Joback Method
cpg	1020.41	J/mol×K	1101.59	Joback Method
cpg	1036.24	J/mol×K	1138.93	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415481&Units=SI

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