Isophthalic acid, butyl 3-phenylpropyl ester

Inchi: InChI=1S/C21H24O4/c1-2-3-14-24-20(22)18-12-7-13-19(16-18)21(23)25-15-8-11-17-9-5
InchiKey: XAIRZZVNJGSSNO-UHFFFAOYSA-N
Formula: C21H24O4
SMILES: CCCCOC(=O)c1cccc(C(=O)OCCCc2ccccc2)c1
Mol. weight [g/mol]: 340.41

Physical Properties

Property code	Value	Unit	Source
gf	-126.71	kJ/mol	Joback Method
hf	-504.78	kJ/mol	Joback Method
hfus	43.41	kJ/mol	Joback Method
hvap	85.87	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.433		Crippen Method
mcvol	274.110	ml/mol	McGowan Method
pc	1606.42	kPa	Joback Method
rinpol	2789.00		NIST Webbook
rinpol	2789.00		NIST Webbook
tb	890.80	K	Joback Method
tc	1113.16	K	Joback Method
tf	536.11	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.31	J/mol×K	890.80	Joback Method
cpg	853.59	J/mol×K	927.86	Joback Method
cpg	866.56	J/mol×K	964.92	Joback Method
cpg	878.28	J/mol×K	1001.98	Joback Method
cpg	888.78	J/mol×K	1039.04	Joback Method
cpg	898.11	J/mol×K	1076.10	Joback Method
cpg	906.31	J/mol×K	1113.16	Joback Method
dvisc	0.0004673	Pa×s	536.11	Joback Method

dvisc	0.0002661	Pa×s	595.23	Joback Method
dvisc	0.0001678	Pa×s	654.34	Joback Method
dvisc	0.0001142	Pa×s	713.45	Joback Method
dvisc	0.0000824	Pa×s	772.57	Joback Method
dvisc	0.0000623	Pa×s	831.68	Joback Method
dvisc	0.0000489	Pa×s	890.80	Joback Method

Sources

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=U344388&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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