Isophthalic acid, butyl 2-methylphenyl ester

Inchi: InChI=1S/C19H20O4/c1-3-4-12-22-18(20)15-9-7-10-16(13-15)19(21)23-17-11-6-5-8-14(1
InchiKey: DKGVYHYLKACLTF-UHFFFAOYSA-N
Formula: C19H20O4
SMILES: CCCCOC(=O)c1cccc(C(=O)Oc2ccccc2C)c1
Mol. weight [g/mol]: 312.36

Physical Properties

Property code	Value	Unit	Source
gf	-153.18	kJ/mol	Joback Method
hf	-474.97	kJ/mol	Joback Method
hfus	37.84	kJ/mol	Joback Method
hvap	82.08	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	4.171		Crippen Method
mcvol	245.930	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	2528.00		NIST Webbook
rinpol	2528.00		NIST Webbook
tb	850.02	K	Joback Method
tc	1076.64	K	Joback Method
tf	526.09	K	Joback Method
vc	0.931	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.25	J/mol×K	850.02	Joback Method
cpg	780.85	J/mol×K	1038.87	Joback Method
cpg	771.74	J/mol×K	1001.10	Joback Method
cpg	761.46	J/mol×K	963.33	Joback Method
cpg	749.97	J/mol×K	925.56	Joback Method
cpg	737.24	J/mol×K	887.79	Joback Method
cpg	788.81	J/mol×K	1076.64	Joback Method
dvisc	0.0000652	Pa×s	850.02	Joback Method

dvisc	0.0000815	Pa×s	796.03	Joback Method
dvisc	0.0001053	Pa×s	742.04	Joback Method
dvisc	0.0001415	Pa×s	688.06	Joback Method
dvisc	0.0002002	Pa×s	634.07	Joback Method
dvisc	0.0003019	Pa×s	580.08	Joback Method
dvisc	0.0004955	Pa×s	526.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344347&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
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

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