Isophthalic acid, butyl 2-formylphenyl ester

Inchi: InChI=1S/C19H18O5/c1-2-3-11-23-18(21)14-8-6-9-15(12-14)19(22)24-17-10-5-4-7-16(17
InchiKey: KWFDQRFRXNLTOU-UHFFFAOYSA-N
Formula: C19H18O5
SMILES: CCCCOC(=O)c1cccc(C(=O)Oc2ccccc2C=O)c1
Mol. weight [g/mol]: 326.34

Physical Properties

Property code	Value	Unit	Source
gf	-252.70	kJ/mol	Joback Method
hf	-560.55	kJ/mol	Joback Method
hfus	40.13	kJ/mol	Joback Method
hvap	88.80	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	3.675		Crippen Method
mcvol	247.500	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
rinpol	2739.00		NIST Webbook
rinpol	2739.00		NIST Webbook
tb	898.68	K	Joback Method
tc	1127.84	K	Joback Method
tf	568.09	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.64	J/mol×K	898.68	Joback Method
cpg	780.47	J/mol×K	1089.65	Joback Method
cpg	773.49	J/mol×K	1051.46	Joback Method
cpg	765.35	J/mol×K	1013.26	Joback Method
cpg	756.01	J/mol×K	975.07	Joback Method
cpg	745.45	J/mol×K	936.87	Joback Method
cpg	786.31	J/mol×K	1127.84	Joback Method
dvisc	0.0000710	Pa×s	898.68	Joback Method

dvisc	0.0000883	Pa×s	843.58	Joback Method
dvisc	0.0001131	Pa×s	788.48	Joback Method
dvisc	0.0001504	Pa×s	733.38	Joback Method
dvisc	0.0002096	Pa×s	678.29	Joback Method
dvisc	0.0003096	Pa×s	623.19	Joback Method
dvisc	0.0004932	Pa×s	568.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344613&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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