Terephthalic acid, ethyl 2-iodobenzyl ester

Inchi: InChI=1S/C17H15IO4/c1-2-21-16(19)12-7-9-13(10-8-12)17(20)22-11-14-5-3-4-6-15(14)1
InchiKey: PVJLQXGRZFQJMT-UHFFFAOYSA-N
Formula: C17H15IO4
SMILES: CCOC(=O)c1ccc(C(=O)OCc2ccccc2I)cc1
Mol. weight [g/mol]: 410.20

Physical Properties

Property code	Value	Unit	Source
gf	-111.90	kJ/mol	Joback Method
hf	-356.82	kJ/mol	Joback Method
hfus	37.07	kJ/mol	Joback Method
hvap	87.00	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	3.825		Crippen Method
mcvol	243.570	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpol	2856.00		NIST Webbook
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tb	897.40	K	Joback Method
tc	1150.26	K	Joback Method
tf	561.61	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.28	J/mol×K	897.40	Joback Method
cpg	696.29	J/mol×K	1108.12	Joback Method
cpg	689.84	J/mol×K	1065.97	Joback Method
cpg	682.25	J/mol×K	1023.83	Joback Method
cpg	673.50	J/mol×K	981.69	Joback Method
cpg	663.53	J/mol×K	939.54	Joback Method
cpg	701.67	J/mol×K	1150.26	Joback Method
dvisc	0.0000638	Pa×s	897.40	Joback Method

dvisc	0.0000795	Pa×s	841.43	Joback Method
dvisc	0.0001022	Pa×s	785.47	Joback Method
dvisc	0.0001366	Pa×s	729.50	Joback Method
dvisc	0.0001915	Pa×s	673.54	Joback Method
dvisc	0.0002855	Pa×s	617.58	Joback Method
dvisc	0.0004608	Pa×s	561.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416071&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