Terephthalic acid, 2-iodobenzyl propyl ester

Inchi: InChI=1S/C18H17IO4/c1-2-11-22-17(20)13-7-9-14(10-8-13)18(21)23-12-15-5-3-4-6-16(1
InchiKey: QPSZNHHHNQELKO-UHFFFAOYSA-N
Formula: C18H17IO4
SMILES: CCCOC(=O)c1ccc(C(=O)OCc2ccccc2I)cc1
Mol. weight [g/mol]: 424.23

Physical Properties

Property code	Value	Unit	Source
gf	-103.48	kJ/mol	Joback Method
hf	-377.46	kJ/mol	Joback Method
hfus	39.66	kJ/mol	Joback Method
hvap	89.22	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	4.215		Crippen Method
mcvol	257.660	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
rinpol	2970.00		NIST Webbook
rinpol	2970.00		NIST Webbook
tb	920.28	K	Joback Method
tc	1169.28	K	Joback Method
tf	572.88	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.27	J/mol×K	920.28	Joback Method
cpg	753.04	J/mol×K	1127.78	Joback Method
cpg	746.43	J/mol×K	1086.28	Joback Method
cpg	738.70	J/mol×K	1044.78	Joback Method
cpg	729.80	J/mol×K	1003.28	Joback Method
cpg	719.67	J/mol×K	961.78	Joback Method
cpg	758.57	J/mol×K	1169.28	Joback Method
dvisc	0.0000552	Pa×s	920.28	Joback Method

dvisc	0.0000690	Pa×s	862.38	Joback Method
dvisc	0.0000891	Pa×s	804.48	Joback Method
dvisc	0.0001197	Pa×s	746.58	Joback Method
dvisc	0.0001689	Pa×s	688.68	Joback Method
dvisc	0.0002540	Pa×s	630.78	Joback Method
dvisc	0.0004149	Pa×s	572.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416072&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