

Terephthalic acid, 2-iodobenzyl pentyl ester

Inchi:	InChI=1S/C20H21IO4/c1-2-3-6-13-24-19(22)15-9-11-16(12-10-15)20(23)25-14-17-7-4-5-
InchiKey:	GCQJVNTNIIHMLGS-UHFFFAOYSA-N
Formula:	C20H21IO4
SMILES:	CCCCCOC(=O)c1ccc(C(=O)OCc2ccccc2I)cc1
Mol. weight [g/mol]:	452.28

Physical Properties

Property code	Value	Unit	Source
gf	-86.64	kJ/mol	Joback Method
hf	-418.74	kJ/mol	Joback Method
hfus	44.84	kJ/mol	Joback Method
hvap	93.67	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	4.995		Crippen Method
mvol	285.840	ml/mol	McGowan Method
pc	1685.18	kPa	Joback Method
rinpol	3186.00		NIST Webbook
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tb	966.04	K	Joback Method
tc	1209.57	K	Joback Method
tf	595.42	K	Joback Method
vc	1.075	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.42	J/mol×K	966.04	Joback Method
cpg	834.03	J/mol×K	1006.63	Joback Method
cpg	844.36	J/mol×K	1047.22	Joback Method
cpg	853.45	J/mol×K	1087.81	Joback Method
cpg	861.37	J/mol×K	1128.40	Joback Method
cpg	868.17	J/mol×K	1168.98	Joback Method
cpg	873.90	J/mol×K	1209.57	Joback Method
dvisc	0.0003330	Paxs	595.42	Joback Method

dvisc	0.0001993	Paxs	657.19	Joback Method
dvisc	0.0001303	Paxs	718.96	Joback Method
dvisc	0.0000912	Paxs	780.73	Joback Method
dvisc	0.0000672	Paxs	842.50	Joback Method
dvisc	0.0000516	Paxs	904.27	Joback Method
dvisc	0.0000410	Paxs	966.04	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=U416074&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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