

Terephthalic acid, hexyl 2-iodobenzyl ester

Inchi:	InChI=1S/C21H23IO4/c1-2-3-4-7-14-25-20(23)16-10-12-17(13-11-16)21(24)26-15-18-8-5
InchiKey:	UPBFOMATGPMVOG-UHFFFAOYSA-N
Formula:	C21H23IO4
SMILES:	CCCCCOC(=O)c1ccc(C(=O)OCc2ccccc2I)cc1
Mol. weight [g/mol]:	466.31

Physical Properties

Property code	Value	Unit	Source
gf	-78.22	kJ/mol	Joback Method
hf	-439.38	kJ/mol	Joback Method
hfus	47.43	kJ/mol	Joback Method
hvap	95.90	kJ/mol	Joback Method
log10ws	-7.31		Crippen Method
logp	5.385		Crippen Method
mvol	299.930	ml/mol	McGowan Method
pc	1559.81	kPa	Joback Method
rinpol	3292.00		NIST Webbook
rinpol	3292.00		NIST Webbook
tb	988.92	K	Joback Method
tc	1230.92	K	Joback Method
tf	606.69	K	Joback Method
vc	1.131	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.47	J/molxK	988.92	Joback Method
cpg	926.51	J/molxK	1190.59	Joback Method
cpg	919.66	J/molxK	1150.26	Joback Method
cpg	911.70	J/molxK	1109.92	Joback Method
cpg	902.55	J/molxK	1069.59	Joback Method
cpg	892.16	J/molxK	1029.25	Joback Method
cpg	932.31	J/molxK	1230.92	Joback Method
dvisc	0.0000353	Paxs	988.92	Joback Method

dvisc	0.0000445	Paxs	925.21	Joback Method
dvisc	0.0000582	Paxs	861.51	Joback Method
dvisc	0.0000793	Paxs	797.81	Joback Method
dvisc	0.0001141	Paxs	734.10	Joback Method
dvisc	0.0001758	Paxs	670.39	Joback Method
dvisc	0.0002969	Paxs	606.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416075&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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