

Terephthalic acid, heptyl 2-iodobenzyl ester

Inchi: InChI=1S/C22H25IO4/c1-2-3-4-5-8-15-26-21(24)17-11-13-18(14-12-17)22(25)27-16-19-9
InchiKey: WIQUCQMCFBIRGX-UHFFFAOYSA-N
Formula: C22H25IO4
SMILES: CCCCCCOC(=O)c1ccc(C(=O)OCc2ccccc2I)cc1
Mol. weight [g/mol]: 480.34

Physical Properties

Property code	Value	Unit	Source
gf	-69.80	kJ/mol	Joback Method
hf	-460.02	kJ/mol	Joback Method
hfus	50.02	kJ/mol	Joback Method
hvap	98.13	kJ/mol	Joback Method
log10ws	-7.73		Crippen Method
logp	5.775		Crippen Method
mvol	314.020	ml/mol	McGowan Method
pc	1447.94	kPa	Joback Method
rinpol	2610.00		NIST Webbook
rinpol	2610.00		NIST Webbook
tb	1011.80	K	Joback Method
tc	1253.13	K	Joback Method
tf	617.96	K	Joback Method
vc	1.188	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	939.11	J/molxK	1011.80	Joback Method
cpg	950.86	J/molxK	1052.02	Joback Method
cpg	961.30	J/molxK	1092.24	Joback Method
cpg	970.48	J/molxK	1132.47	Joback Method
cpg	978.49	J/molxK	1172.69	Joback Method
cpg	985.37	J/molxK	1212.91	Joback Method
cpg	991.19	J/molxK	1253.13	Joback Method
dvisc	0.0002640	Paxs	617.96	Joback Method

dvisc	0.0001547	Paxs	683.60	Joback Method
dvisc	0.0000996	Paxs	749.24	Joback Method
dvisc	0.0000688	Paxs	814.88	Joback Method
dvisc	0.0000502	Paxs	880.52	Joback Method
dvisc	0.0000383	Paxs	946.16	Joback Method
dvisc	0.0000303	Paxs	1011.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416076&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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