Sebacic acid, di(4-iodobenzyl) ester

Inchi: InChI=1S/C24H28I2O4/c25-21-13-9-19(10-14-21)17-29-23(27)7-5-3-1-2-4-6-8-24(28)30-

InchiKey: XKCDVIUBMFPZKE-UHFFFAOYSA-N

Formula: C24H28I2O4

SMILES: O=C(CCCCCCCCC(=O)OCc1ccc(I)cc1)OCc1ccc(I)cc1

Mol. weight [g/mol]: 634.29

Physical Properties

Property code	Value	Unit	Source
gf	5.16	kJ/mol	Joback Method
hf	-424.43	kJ/mol	Joback Method
hfus	59.61	kJ/mol	Joback Method
hvap	111.95	kJ/mol	Joback Method
log10ws	-9.09		Crippen Method
logp	6.803		Crippen Method
mcvol	368.020	ml/mol	McGowan Method
pc	1238.09	kPa	Joback Method
rinpol	3719.00		NIST Webbook
rinpol	3719.00		NIST Webbook
tb	1150.70	K	Joback Method
tc	1412.68	K	Joback Method
tf	698.56	K	Joback Method
vc	1.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1092.82	J/mol×K	1150.70	Joback Method
cpg	1102.90	J/mol×K	1194.36	Joback Method
cpg	1111.83	J/mol×K	1238.03	Joback Method
cpg	1119.75	J/mol×K	1281.69	Joback Method
cpg	1126.76	J/mol×K	1325.35	Joback Method
cpg	1132.97	J/mol×K	1369.02	Joback Method
cpg	1138.51	J/mol×K	1412.68	Joback Method
dvisc	0.0001327	Pa×s	698.56	Joback Method

dvisc	0.0000762	Pa×s	773.92	Joback Method
dvisc	0.0000483	Pa×s	849.27	Joback Method
dvisc	0.0000329	Pa×s	924.63	Joback Method
dvisc	0.0000238	Pa×s	999.99	Joback Method
dvisc	0.0000180	Pa×s	1075.34	Joback Method
dvisc	0.0000141	Pa×s	1150.70	Joback Method

Sources

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=U380632&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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