

Sebacic acid, di(3-iodobenzyl) ester

Inchi: InChI=1S/C24H28I2O4/c25-21-11-7-9-19(15-21)17-29-23(27)13-5-3-1-2-4-6-14-24(28)30
InchiKey: KUNACYHMENOTNQ-UHFFFAOYSA-N
Formula: C24H28I2O4
SMILES: O=C(CCCCCCCCC(=O)OCc1cccc(I)c1)OCc1cccc(I)c1
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
mvol	368.020	ml/mol	McGowan Method
pc	1238.09	kPa	Joback Method
rinpol	3570.00		NIST Webbook
rinpol	3570.00		NIST Webbook
tb	1150.70	K	Joback Method
tc	1412.68	K	Joback Method
tf	698.56	K	Joback Method
vc	1.387	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0000762	Paxs	773.92	Joback Method
dvisc	0.0000483	Paxs	849.27	Joback Method
dvisc	0.0000329	Paxs	924.63	Joback Method
dvisc	0.0000238	Paxs	999.99	Joback Method
dvisc	0.0000180	Paxs	1075.34	Joback Method
dvisc	0.0000141	Paxs	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=U380759&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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