

Sebacic acid, isohexyl phenyl ester

Inchi:	InChI=1S/C22H34O4/c1-19(2)13-12-18-25-21(23)16-10-5-3-4-6-11-17-22(24)26-20-14-8
InchiKey:	PCTMWAQVWPNSHM-UHFFFAOYSA-N
Formula:	C22H34O4
SMILES:	CC(C)CCCOC(=O)CCCCCCCC(=O)Oc1ccccc1
Mol. weight [g/mol]:	362.50

Physical Properties

Property code	Value	Unit	Source
gf	-223.51	kJ/mol	Joback Method
hf	-755.76	kJ/mol	Joback Method
hfus	48.83	kJ/mol	Joback Method
hvap	84.77	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.692		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1189.88	kPa	Joback Method
rinpol	2722.00		NIST Webbook
tb	881.58	K	Joback Method
tc	1084.93	K	Joback Method
tf	493.44	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.33	J/molxK	881.58	Joback Method
cpg	1015.04	J/molxK	915.47	Joback Method
cpg	1030.51	J/molxK	949.36	Joback Method
cpg	1044.77	J/molxK	983.26	Joback Method
cpg	1057.86	J/molxK	1017.15	Joback Method
cpg	1069.80	J/molxK	1051.04	Joback Method
cpg	1080.63	J/molxK	1084.93	Joback Method
dvisc	0.0006396	Paxs	493.44	Joback Method
dvisc	0.0003024	Paxs	558.13	Joback Method

dvisc	0.0001670	Paxs	622.82	Joback Method
dvisc	0.0001031	Paxs	687.51	Joback Method
dvisc	0.0000692	Paxs	752.20	Joback Method
dvisc	0.0000495	Paxs	816.89	Joback Method
dvisc	0.0000371	Paxs	881.58	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=U354509&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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