

Sebacic acid, isobutyl 2-phenylphenyl ester

Inchi:	InChI=1S/C26H34O4/c1-21(2)20-29-25(27)18-10-5-3-4-6-11-19-26(28)30-24-17-13-12-1
InchiKey:	OFNBLOCUWXSJST-UHFFFAOYSA-N
Formula:	C26H34O4
SMILES:	CC(C)COC(=O)CCCCCCCC(=O)Oc1ccccc1-c1ccccc1
Mol. weight [g/mol]:	410.55

Physical Properties

Property code	Value	Unit	Source
gf	-87.05	kJ/mol	Joback Method
hf	-613.26	kJ/mol	Joback Method
hfus	52.84	kJ/mol	Joback Method
hvap	96.61	kJ/mol	Joback Method
log10ws	-8.03		Crippen Method
logp	6.579		Crippen Method
mvol	344.560	ml/mol	McGowan Method
pc	1135.96	kPa	Joback Method
rmpol	3020.00		NIST Webbook
tb	1004.76	K	Joback Method
tc	1232.71	K	Joback Method
tf	577.46	K	Joback Method
vc	1.317	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1138.11	J/molxK	1004.76	Joback Method
cpg	1152.68	J/molxK	1042.75	Joback Method
cpg	1165.77	J/molxK	1080.74	Joback Method
cpg	1177.42	J/molxK	1118.73	Joback Method
cpg	1187.72	J/molxK	1156.72	Joback Method
cpg	1196.72	J/molxK	1194.72	Joback Method
cpg	1204.48	J/molxK	1232.71	Joback Method
dvisc	0.0002930	Paxs	577.46	Joback Method
dvisc	0.0001492	Paxs	648.68	Joback Method

dvisc	0.0000869	Paxs	719.89	Joback Method
dvisc	0.0000557	Paxs	791.11	Joback Method
dvisc	0.0000385	Paxs	862.33	Joback Method
dvisc	0.0000281	Paxs	933.54	Joback Method
dvisc	0.0000215	Paxs	1004.76	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=U355064&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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