Sebacic acid, di(2-acetylphenyl) ester

Inchi: InChI=1S/C26H30O6/c1-19(27)21-13-9-11-15-23(21)31-25(29)17-7-5-3-4-6-8-18-26(30)3
InchiKey: MSKCJRWMWHHQJW-UHFFFAOYSA-N
Formula: C26H30O6
SMILES: CC(=O)c1ccccc1OC(=O)CCCCCCCCC(=O)Oc1ccccc1C(C)=O
Mol. weight [g/mol]: 438.51

Physical Properties

Property code	Value	Unit	Source
gf	-352.08	kJ/mol	Joback Method
hf	-844.61	kJ/mol	Joback Method
hfus	59.17	kJ/mol	Joback Method
hvap	111.15	kJ/mol	Joback Method
log10ws	-7.58		Crippen Method
logp	5.724		Crippen Method
mcvol	347.700	ml/mol	McGowan Method
pc	1219.14	kPa	Joback Method
rinpol	3190.00		NIST Webbook
tb	1117.92	K	Joback Method
tc	1368.69	K	Joback Method
tf	704.84	K	Joback Method
vc	1.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1147.34	J/mol×K	1117.92	Joback Method
cpg	1156.89	J/mol×K	1159.72	Joback Method
cpg	1164.74	J/mol×K	1201.51	Joback Method
cpg	1170.95	J/mol×K	1243.31	Joback Method
cpg	1175.59	J/mol×K	1285.10	Joback Method
cpg	1178.73	J/mol×K	1326.90	Joback Method
cpg	1180.43	J/mol×K	1368.69	Joback Method
dvisc	0.0001696	Pa×s	704.84	Joback Method
dvisc	0.0001030	Pa×s	773.69	Joback Method

dvisc	0.0000679	Pa×s	842.53	Joback Method
dvisc	0.0000476	Pa×s	911.38	Joback Method
dvisc	0.0000351	Pa×s	980.23	Joback Method
dvisc	0.0000269	Pa×s	1049.07	Joback Method
dvisc	0.0000214	Pa×s	1117.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354976&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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