Sebacic acid, heptyl 4-isopropoxyphenyl ester

Inchi: InChI=1S/C26H42O5/c1-4-5-6-11-14-21-29-25(27)15-12-9-7-8-10-13-16-26(28)31-24-19
InchiKey: LKFMZSZNEILWBV-UHFFFAOYSA-N
Formula: C26H42O5
SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(OC(C)C)cc1
Mol. weight [g/mol]: 434.61

Physical Properties

Property code	Value	Unit	Source
gf	-304.46	kJ/mol	Joback Method
hf	-982.01	kJ/mol	Joback Method
hfus	59.99	kJ/mol	Joback Method
hvap	96.74	kJ/mol	Joback Method
log10ws	-8.00		Crippen Method
logp	7.014		Crippen Method
mcvol	374.190	ml/mol	McGowan Method
pc	909.98	kPa	Joback Method
rinpol	3120.00		NIST Webbook
tb	1000.50	K	Joback Method
tc	1226.12	K	Joback Method
tf	573.27	K	Joback Method
vc	1.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1273.44	J/mol×K	1000.50	Joback Method
cpg	1339.48	J/mol×K	1188.52	Joback Method
cpg	1329.67	J/mol×K	1150.91	Joback Method
cpg	1318.19	J/mol×K	1113.31	Joback Method
cpg	1305.02	J/mol×K	1075.71	Joback Method
cpg	1290.12	J/mol×K	1038.10	Joback Method
cpg	1347.66	J/mol×K	1226.12	Joback Method
dvisc	0.0000153	Pa×s	1000.50	Joback Method
dvisc	0.0000202	Pa×s	929.29	Joback Method

dvisc	0.0000279	Pa×s	858.09	Joback Method
dvisc	0.0000409	Pa×s	786.88	Joback Method
dvisc	0.0000649	Pa×s	715.68	Joback Method
dvisc	0.0001137	Pa×s	644.47	Joback Method
dvisc	0.0002292	Pa×s	573.27	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=U354408&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