Sebacic acid, isobutyl 4-methoxyphenyl ester

Inchi: InChI=1S/C21H32O5/c1-17(2)16-25-20(22)10-8-6-4-5-7-9-11-21(23)26-19-14-12-18(24-3
InchiKey: FNOCFXGLQBSRHC-UHFFFAOYSA-N
Formula: C21H32O5
SMILES: COc1ccc(OC(=O)CCCCCCCCC(=O)OCC(C)C)cc1
Mol. weight [g/mol]: 364.48

Physical Properties

Property code	Value	Unit	Source
gf	-346.56	kJ/mol	Joback Method
hf	-878.81	kJ/mol	Joback Method
hfus	47.04	kJ/mol	Joback Method
hvap	85.61	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	4.921		Crippen Method
mcvol	303.740	ml/mol	McGowan Method
pc	1244.21	kPa	Joback Method
rinpol	2780.00		NIST Webbook
rinpol	2780.00		NIST Webbook
tb	886.10	K	Joback Method
tc	1090.63	K	Joback Method
tf	516.92	K	Joback Method
vc	1.163	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.23	J/mol×K	886.10	Joback Method
cpg	983.12	J/mol×K	920.19	Joback Method
cpg	997.70	J/mol×K	954.28	Joback Method
cpg	1011.00	J/mol×K	988.37	Joback Method
cpg	1023.03	J/mol×K	1022.46	Joback Method
cpg	1033.79	J/mol×K	1056.54	Joback Method
cpg	1043.30	J/mol×K	1090.63	Joback Method
dvisc	0.0004176	Pa×s	516.92	Joback Method

dvisc	0.0002177	Pa×s	578.45	Joback Method
dvisc	0.0001286	Pa×s	639.98	Joback Method
dvisc	0.0000833	Pa×s	701.51	Joback Method
dvisc	0.0000579	Pa×s	763.04	Joback Method
dvisc	0.0000425	Pa×s	824.57	Joback Method
dvisc	0.0000325	Pa×s	886.10	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=U354773&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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