Sebacic acid, butyl 2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C22H34O6/c1-4-5-17-27-20(23)15-10-8-6-7-9-11-16-21(24)28-22-18(25-2)13-1

InchiKey: IVOMTCLFYAWFAG-UHFFFAOYSA-N

Formula: C22H34O6

SMILES: CCCCOC(=O)CCCCCCCCC(=O)Oc1c(OC)cccc1OC

Mol. weight [g/mol]: 394.50

Physical Properties

Property code	Value	Unit	Source
gf	-450.33	kJ/mol	Joback Method
hf	-1037.86	kJ/mol	Joback Method
hfus	53.95	kJ/mol	Joback Method
hvap	91.30	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	5.073		Crippen Method
mcvol	323.700	ml/mol	McGowan Method
pc	1132.91	kPa	Joback Method
rinpol	2936.00		NIST Webbook
tb	936.82	K	Joback Method
tc	1147.59	K	Joback Method
tf	577.94	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1055.48	J/mol×K	936.82	Joback Method
cpg	1070.70	J/mol×K	971.95	Joback Method
cpg	1084.40	J/mol×K	1007.08	Joback Method
cpg	1096.55	J/mol×K	1042.20	Joback Method
cpg	1107.18	J/mol×K	1077.33	Joback Method
cpg	1116.26	J/mol×K	1112.46	Joback Method
cpg	1123.79	J/mol×K	1147.59	Joback Method
dvisc	0.0002064	Pa×s	577.94	Joback Method
dvisc	0.0001210	Pa×s	637.75	Joback Method

dvisc	0.0000777	Pa×s	697.57	Joback Method
dvisc	0.0000535	Pa×s	757.38	Joback Method
dvisc	0.0000389	Pa×s	817.19	Joback Method
dvisc	0.0000296	Pa×s	877.01	Joback Method
dvisc	0.0000233	Pa×s	936.82	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354751&Units=SI

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