Sebacic acid, (1,3-benzodioxol-5-yl)methyl butyl ester

Inchi: InChI=1S/C22H32O6/c1-2-3-14-25-21(23)10-8-6-4-5-7-9-11-22(24)26-16-18-12-13-19-20

InchiKey: MLBIREAQRPGEHI-UHFFFAOYSA-N

Formula: C22H32O6

SMILES: CCCCOC(=O)CCCCCCCCC(=O)OCc1ccc2c(c1)OCO2

Mol. weight [g/mol]: 392.49

Physical Properties

Property code	Value	Unit	Source
gf	-344.11	kJ/mol	Joback Method
hf	-944.28	kJ/mol	Joback Method
hfus	64.59	kJ/mol	Joback Method
hvap	95.72	kJ/mol	Joback Method
log10ws	-6.15		Crippen Method
logp	4.923		Crippen Method
mcvol	312.840	ml/mol	McGowan Method
pc	1282.83	kPa	Joback Method
rinpol	2931.00		NIST Webbook
rinpol	2931.00		NIST Webbook
tb	957.29	K	Joback Method
tc	1173.74	K	Joback Method
tf	608.80	K	Joback Method
vc	1.208	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1039.25	J/mol×K	957.29	Joback Method
cpg	1054.25	J/mol×K	993.37	Joback Method
cpg	1068.11	J/mol×K	1029.44	Joback Method
cpg	1080.90	J/mol×K	1065.52	Joback Method
cpg	1092.67	J/mol×K	1101.59	Joback Method
cpg	1103.48	J/mol×K	1137.67	Joback Method
cpg	1113.39	J/mol×K	1173.74	Joback Method
dvisc	0.0005163	Pa×s	608.80	Joback Method

dvisc	0.0003250	Pa×s	666.88	Joback Method
dvisc	0.0002204	Pa×s	724.96	Joback Method
dvisc	0.0001583	Pa×s	783.04	Joback Method
dvisc	0.0001190	Pa×s	841.13	Joback Method
dvisc	0.0000928	Pa×s	899.21	Joback Method
dvisc	0.0000746	Pa×s	957.29	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=U380688&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