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

Inchi: InChI=1S/C22H32O6/c1-17(2)14-25-21(23)9-7-5-3-4-6-8-10-22(24)26-15-18-11-12-19-20

InchiKey: JIBUTEMOLZBQPK-UHFFFAOYSA-N

Formula: C22H32O6

SMILES: CC(C)COC(=O)CCCCCCCCC(=O)OCc1ccc2c(c1)OCO2

Mol. weight [g/mol]: 392.49

Physical Properties

Property code	Value	Unit	Source
gf	-346.55	kJ/mol	Joback Method
hf	-949.56	kJ/mol	Joback Method
hfus	61.07	kJ/mol	Joback Method
hvap	95.33	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	4.778		Crippen Method
mcvol	312.840	ml/mol	McGowan Method
pc	1290.21	kPa	Joback Method
rinpol	2893.00		NIST Webbook
rinpol	2893.00		NIST Webbook
tb	956.85	K	Joback Method
tc	1174.01	K	Joback Method
tf	593.80	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1039.67	J/mol×K	956.85	Joback Method
cpg	1103.70	J/mol×K	1137.82	Joback Method
cpg	1092.97	J/mol×K	1101.62	Joback Method
cpg	1081.26	J/mol×K	1065.43	Joback Method
cpg	1068.51	J/mol×K	1029.24	Joback Method
cpg	1054.67	J/mol×K	993.04	Joback Method
cpg	1113.51	J/mol×K	1174.01	Joback Method
dvisc	0.0000680	Pa×s	956.85	Joback Method

dvisc	0.0000857	Pa×s	896.34	Joback Method
dvisc	0.0001116	Pa×s	835.83	Joback Method
dvisc	0.0001515	Pa×s	775.32	Joback Method
dvisc	0.0002165	Pa×s	714.82	Joback Method
dvisc	0.0003306	Pa×s	654.31	Joback Method
dvisc	0.0005504	Pa×s	593.80	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=U380687&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