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

Inchi: InChI=1S/C26H30O8/c27-25(29-15-19-9-11-21-23(13-19)33-17-31-21)7-5-3-1-2-4-6-8-26
InchiKey: BLOJYYXMNWMWMI-UHFFFAOYSA-N
Formula: C26H30O8
SMILES: O=C(CCCCCCCCC(=O)OCc1ccc2c(c1)OCO2)OCc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 470.51

Physical Properties

Property code	Value	Unit	Source
gf	-321.06	kJ/mol	Joback Method
hf	-984.11	kJ/mol	Joback Method
hfus	81.24	kJ/mol	Joback Method
hvap	117.47	kJ/mol	Joback Method
log10ws	-7.21		Crippen Method
logp	5.051		Crippen Method
mcvol	346.320	ml/mol	McGowan Method
pc	1341.76	kPa	Joback Method
rinpol	3505.00		NIST Webbook
rinpol	3505.00		NIST Webbook
tb	1150.76	K	Joback Method
tc	1409.04	K	Joback Method
tf	780.66	K	Joback Method
vc	1.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1206.69	J/mol×K	1150.76	Joback Method
cpg	1220.34	J/mol×K	1193.81	Joback Method
cpg	1233.28	J/mol×K	1236.85	Joback Method
cpg	1245.65	J/mol×K	1279.90	Joback Method
cpg	1257.62	J/mol×K	1322.94	Joback Method
cpg	1269.36	J/mol×K	1365.99	Joback Method
cpg	1281.03	J/mol×K	1409.04	Joback Method
dvisc	0.0003773	Pa×s	780.66	Joback Method

dvisc	0.0002659	Pa×s	842.34	Joback Method
dvisc	0.0001966	Pa×s	904.03	Joback Method
dvisc	0.0001511	Pa×s	965.71	Joback Method
dvisc	0.0001198	Pa×s	1027.39	Joback Method
dvisc	0.0000976	Pa×s	1089.08	Joback Method
dvisc	0.0000812	Pa×s	1150.76	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=U380692&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

Latest version available from:
https://www.chemeo.com/cid/91-473-6/Sebacic-acid-di-1-3-benzodioxol-5-yl-methyl-ester.pdf
Generated by Cheméo on 2024-04-25 20:31:03.752604255 +0000 UTC m=+16366312.673181578.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.