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

Inchi: InChI=1S/C21H30O6/c1-2-13-24-20(22)9-7-5-3-4-6-8-10-21(23)25-15-17-11-12-18-19(14

InchiKey: ZKGMGNMCPMDJAQ-UHFFFAOYSA-N

Formula: C21H30O6

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

Mol. weight [g/mol]: 378.46

Physical Properties

Property code	Value	Unit	Source
gf	-352.53	kJ/mol	Joback Method
hf	-923.64	kJ/mol	Joback Method
hfus	62.00	kJ/mol	Joback Method
hvap	93.49	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	4.532		Crippen Method
mcvol	298.750	ml/mol	McGowan Method
pc	1375.82	kPa	Joback Method
rinpol	2839.00		NIST Webbook
rinpol	2839.00		NIST Webbook
tb	934.41	K	Joback Method
tc	1148.05	K	Joback Method
tf	597.53	K	Joback Method
vc	1.151	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	979.05	J/mol×K	934.41	Joback Method
cpg	993.76	J/mol×K	970.02	Joback Method
cpg	1007.37	J/mol×K	1005.62	Joback Method
cpg	1019.94	J/mol×K	1041.23	Joback Method
cpg	1031.53	J/mol×K	1076.84	Joback Method
cpg	1042.18	J/mol×K	1112.44	Joback Method
cpg	1051.96	J/mol×K	1148.05	Joback Method
dvisc	0.0005737	Pa×s	597.53	Joback Method

dvisc	0.0003652	Pa×s	653.68	Joback Method
dvisc	0.0002498	Pa×s	709.82	Joback Method
dvisc	0.0001806	Pa×s	765.97	Joback Method
dvisc	0.0001365	Pa×s	822.12	Joback Method
dvisc	0.0001069	Pa×s	878.26	Joback Method
dvisc	0.0000862	Pa×s	934.41	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=U380686&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

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