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

Inchi: InChI=1S/C23H34O6/c1-2-3-10-15-26-22(24)11-8-6-4-5-7-9-12-23(25)27-17-19-13-14-20

InchiKey: YCUSZKPZERPQSY-UHFFFAOYSA-N

Formula: C23H34O6

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

Mol. weight [g/mol]: 406.51

Physical Properties

Property code	Value	Unit	Source
gf	-335.69	kJ/mol	Joback Method
hf	-964.92	kJ/mol	Joback Method
hfus	67.19	kJ/mol	Joback Method
hvap	97.95	kJ/mol	Joback Method
log10ws	-6.57		Crippen Method
logp	5.313		Crippen Method
mcvol	326.930	ml/mol	McGowan Method
pc	1198.96	kPa	Joback Method
rinpol	3011.00		NIST Webbook
rinpol	3011.00		NIST Webbook
tb	980.17	K	Joback Method
tc	1200.38	K	Joback Method
tf	620.07	K	Joback Method
vc	1.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1100.05	J/mol×K	980.17	Joback Method
cpg	1165.44	J/mol×K	1163.68	Joback Method
cpg	1154.47	J/mol×K	1126.98	Joback Method
cpg	1142.51	J/mol×K	1090.27	Joback Method
cpg	1129.50	J/mol×K	1053.57	Joback Method
cpg	1115.36	J/mol×K	1016.87	Joback Method
cpg	1175.48	J/mol×K	1200.38	Joback Method
dvisc	0.0000644	Pa×s	980.17	Joback Method

dvisc	0.0000804	Pa×s	920.15	Joback Method
dvisc	0.0001035	Pa×s	860.14	Joback Method
dvisc	0.0001384	Pa×s	800.12	Joback Method
dvisc	0.0001939	Pa×s	740.10	Joback Method
dvisc	0.0002884	Pa×s	680.09	Joback Method
dvisc	0.0004632	Pa×s	620.07	Joback Method

Sources

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=U380689&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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