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

Inchi: InChI=1S/C20H28O6/c1-2-23-19(21)9-7-5-3-4-6-8-10-20(22)24-14-16-11-12-17-18(13-16

InchiKey: FZUSCKHKENYCMJ-UHFFFAOYSA-N

Formula: C20H28O6

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

Mol. weight [g/mol]: 364.43

Physical Properties

Property code	Value	Unit	Source
gf	-360.95	kJ/mol	Joback Method
hf	-903.00	kJ/mol	Joback Method
hfus	59.41	kJ/mol	Joback Method
hvap	91.27	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.142		Crippen Method
mcvol	284.660	ml/mol	McGowan Method
pc	1479.29	kPa	Joback Method
rinpol	2737.00		NIST Webbook
rinpol	2737.00		NIST Webbook
tb	911.53	K	Joback Method
tc	1123.24	K	Joback Method
tf	586.26	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	919.49	J/mol×K	911.53	Joback Method
cpg	981.57	J/mol×K	1087.95	Joback Method
cpg	971.08	J/mol×K	1052.67	Joback Method
cpg	959.67	J/mol×K	1017.38	Joback Method
cpg	947.30	J/mol×K	982.10	Joback Method
cpg	933.93	J/mol×K	946.81	Joback Method
cpg	991.21	J/mol×K	1123.24	Joback Method
dvisc	0.0000994	Pa×s	911.53	Joback Method

dvisc	0.0001228	Pa×s	857.32	Joback Method
dvisc	0.0001561	Pa×s	803.11	Joback Method
dvisc	0.0002054	Pa×s	748.89	Joback Method
dvisc	0.0002822	Pa×s	694.68	Joback Method
dvisc	0.0004090	Pa×s	640.47	Joback Method
dvisc	0.0006350	Pa×s	586.26	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=U380685&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