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

Inchi: InChI=1S/C25H38O6/c1-2-3-4-9-12-17-28-24(26)13-10-7-5-6-8-11-14-25(27)29-19-21-15
InchiKey: AOPKLNYIRDCWIW-UHFFFAOYSA-N
Formula: C25H38O6
SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)OCc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 434.57

Physical Properties

Property code	Value	Unit	Source
gf	-318.85	kJ/mol	Joback Method
hf	-1006.20	kJ/mol	Joback Method
hfus	72.36	kJ/mol	Joback Method
hvap	102.40	kJ/mol	Joback Method
log10ws	-7.40		Crippen Method
logp	6.093		Crippen Method
mcvol	355.110	ml/mol	McGowan Method
pc	1054.14	kPa	Joback Method
rinpol	3151.00		NIST Webbook
rinpol	3151.00		NIST Webbook
tb	1025.93	K	Joback Method
tc	1256.76	K	Joback Method
tf	642.61	K	Joback Method
vc	1.375	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1223.25	J/mol×K	1025.93	Joback Method
cpg	1291.28	J/mol×K	1218.29	Joback Method
cpg	1279.95	J/mol×K	1179.81	Joback Method
cpg	1267.57	J/mol×K	1141.34	Joback Method
cpg	1254.05	J/mol×K	1102.87	Joback Method
cpg	1239.30	J/mol×K	1064.40	Joback Method
cpg	1301.63	J/mol×K	1256.76	Joback Method
dvisc	0.0000478	Pa×s	1025.93	Joback Method

dvisc	0.0000600	Pa×s	962.04	Joback Method
dvisc	0.0000778	Pa×s	898.16	Joback Method
dvisc	0.0001050	Pa×s	834.27	Joback Method
dvisc	0.0001490	Pa×s	770.38	Joback Method
dvisc	0.0002251	Pa×s	706.50	Joback Method
dvisc	0.0003693	Pa×s	642.61	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=U380691&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