Sebacic acid, 4-methoxybenzyl octyl ester

Inchi: InChI=1S/C26H42O5/c1-3-4-5-6-11-14-21-30-25(27)15-12-9-7-8-10-13-16-26(28)31-22-2
InchiKey: NESSUINXQIXGNF-UHFFFAOYSA-N
Formula: C26H42O5
SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)OCc1ccc(OC)cc1
Mol. weight [g/mol]: 434.61

Physical Properties

Property code	Value	Unit	Source
gf	-302.02	kJ/mol	Joback Method
hf	-976.73	kJ/mol	Joback Method
hfus	63.51	kJ/mol	Joback Method
hvap	97.13	kJ/mol	Joback Method
log10ws	-7.73		Crippen Method
logp	6.763		Crippen Method
mcvol	374.190	ml/mol	McGowan Method
pc	905.61	kPa	Joback Method
rinpol	3319.00		NIST Webbook
rinpol	3319.00		NIST Webbook
tb	1000.94	K	Joback Method
tc	1227.37	K	Joback Method
tf	588.27	K	Joback Method
vc	1.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1273.11	J/mol×K	1000.94	Joback Method
cpg	1289.90	J/mol×K	1038.68	Joback Method
cpg	1304.93	J/mol×K	1076.42	Joback Method
cpg	1318.22	J/mol×K	1114.15	Joback Method
cpg	1329.82	J/mol×K	1151.89	Joback Method
cpg	1339.75	J/mol×K	1189.63	Joback Method
cpg	1348.07	J/mol×K	1227.37	Joback Method
dvisc	0.0002091	Pa×s	588.27	Joback Method

dvisc	0.0001102	Pa×s	657.05	Joback Method
dvisc	0.0000656	Pa×s	725.83	Joback Method
dvisc	0.0000427	Pa×s	794.61	Joback Method
dvisc	0.0000298	Pa×s	863.38	Joback Method
dvisc	0.0000219	Pa×s	932.16	Joback Method
dvisc	0.0000168	Pa×s	1000.94	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U354367&Units=SI

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