Sebacic acid, di(2-methoxybenzyl) ester

Inchi: InChI=1S/C26H34O6/c1-29-23-15-11-9-13-21(23)19-31-25(27)17-7-5-3-4-6-8-18-26(28)3
InchiKey: DALHIKSHZZZEQW-UHFFFAOYSA-N
Formula: C26H34O6
SMILES: COc1ccccc1COC(=O)CCCCCCCCC(=O)OCc1ccccc1OC
Mol. weight [g/mol]: 442.54

Physical Properties

Property code	Value	Unit	Source
gf	-304.24	kJ/mol	Joback Method
hf	-883.89	kJ/mol	Joback Method
hfus	58.35	kJ/mol	Joback Method
hvap	102.48	kJ/mol	Joback Method
log10ws	-7.03		Crippen Method
logp	5.611		Crippen Method
mcvol	356.300	ml/mol	McGowan Method
pc	1093.54	kPa	Joback Method
rinpol	3292.00		NIST Webbook
rinpol	3292.00		NIST Webbook
tb	1055.02	K	Joback Method
tc	1291.64	K	Joback Method
tf	649.44	K	Joback Method
vc	1.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1189.62	J/mol×K	1055.02	Joback Method
cpg	1201.58	J/mol×K	1094.46	Joback Method
cpg	1211.57	J/mol×K	1133.89	Joback Method
cpg	1219.62	J/mol×K	1173.33	Joback Method
cpg	1225.73	J/mol×K	1212.77	Joback Method
cpg	1229.95	J/mol×K	1252.20	Joback Method
cpg	1232.28	J/mol×K	1291.64	Joback Method
dvisc	0.0001178	Pa×s	649.44	Joback Method

dvisc	0.0000688	Pa×s	717.04	Joback Method
dvisc	0.0000441	Pa×s	784.63	Joback Method
dvisc	0.0000303	Pa×s	852.23	Joback Method
dvisc	0.0000220	Pa×s	919.83	Joback Method
dvisc	0.0000167	Pa×s	987.42	Joback Method
dvisc	0.0000132	Pa×s	1055.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380778&Units=SI
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

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