Sebacic acid, heptyl 1-phenylpropyl ester

Inchi: InChI=1S/C26H42O4/c1-3-5-6-11-17-22-29-25(27)20-15-9-7-8-10-16-21-26(28)30-24(4-2
InchiKey: KAFYOGQIFIUKIQ-UHFFFAOYSA-N
Formula: C26H42O4
SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)OC(CC)c1ccccc1
Mol. weight [g/mol]: 418.61

Physical Properties

Property code	Value	Unit	Source
gf	-189.83	kJ/mol	Joback Method
hf	-838.32	kJ/mol	Joback Method
hfus	59.19	kJ/mol	Joback Method
hvap	93.67	kJ/mol	Joback Method
log10ws	-7.99		Crippen Method
logp	7.315		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	927.81	kPa	Joback Method
rinpol	2961.00		NIST Webbook
tb	973.10	K	Joback Method
tc	1191.51	K	Joback Method
tf	538.52	K	Joback Method
vc	1.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1244.58	J/mol×K	973.10	Joback Method
cpg	1318.03	J/mol×K	1155.11	Joback Method
cpg	1306.16	J/mol×K	1118.71	Joback Method
cpg	1292.93	J/mol×K	1082.30	Joback Method
cpg	1278.29	J/mol×K	1045.90	Joback Method
cpg	1262.19	J/mol×K	1009.50	Joback Method
cpg	1328.62	J/mol×K	1191.51	Joback Method
dvisc	0.0000203	Pa×s	973.10	Joback Method
dvisc	0.0000272	Pa×s	900.67	Joback Method

dvisc	0.0000385	Pa×s	828.24	Joback Method
dvisc	0.0000582	Pa×s	755.81	Joback Method
dvisc	0.0000959	Pa×s	683.38	Joback Method
dvisc	0.0001780	Pa×s	610.95	Joback Method
dvisc	0.0003904	Pa×s	538.52	Joback Method

Sources

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=U354991&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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