Sebacic acid, isobutyl 4-phenylphenyl ester

Inchi: InChI=1S/C26H34O4/c1-21(2)20-29-25(27)14-10-5-3-4-6-11-15-26(28)30-24-18-16-23(1
InchiKey: WTPSPOGMEPKVAN-UHFFFAOYSA-N
Formula: C26H34O4
SMILES: CC(C)COC(=O)CCCCCCCCC(=O)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 410.55

Physical Properties

Property code	Value	Unit	Source
gf	-87.05	kJ/mol	Joback Method
hf	-613.26	kJ/mol	Joback Method
hfus	52.84	kJ/mol	Joback Method
hvap	96.61	kJ/mol	Joback Method
log10ws	-8.03		Crippen Method
logp	6.579		Crippen Method
mcvol	344.560	ml/mol	McGowan Method
pc	1135.96	kPa	Joback Method
rinpol	3307.00		NIST Webbook
rinpol	3307.00		NIST Webbook
tb	1004.76	K	Joback Method
tc	1232.71	K	Joback Method
tf	577.46	K	Joback Method
vc	1.317	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1138.11	J/mol×K	1004.76	Joback Method
cpg	1196.72	J/mol×K	1194.72	Joback Method
cpg	1187.72	J/mol×K	1156.72	Joback Method
cpg	1177.42	J/mol×K	1118.73	Joback Method
cpg	1165.77	J/mol×K	1080.74	Joback Method
cpg	1152.68	J/mol×K	1042.75	Joback Method
cpg	1204.48	J/mol×K	1232.71	Joback Method
dvisc	0.0000215	Pa×s	1004.76	Joback Method

dvisc	0.0000281	Pa×s	933.54	Joback Method
dvisc	0.0000385	Pa×s	862.33	Joback Method
dvisc	0.0000557	Pa×s	791.11	Joback Method
dvisc	0.0000869	Pa×s	719.89	Joback Method
dvisc	0.0001492	Pa×s	648.68	Joback Method
dvisc	0.0002930	Pa×s	577.46	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=U355251&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